Propanoic acid, decyl ester

Other names:	n-Decyl propanoate
	Decyl propionate
	Propionic acid, decyl ester
	n-Decyl n-propionate
Inchi:	InChI=1S/C13H26O2/c1-3-5-6-7-8-9-10-11-12-15-13(14)4-2/h3-12H2,1-2H3
InchiKey:	HUOYUOXEIKDMFT-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCCCCOC(=O)CC
Mol. weight [g/mol]:	214.34
CAS:	5454-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-556.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1478.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1480.05		NIST Webbook
rinpol	1501.10		NIST Webbook
rinpol	1476.00		NIST Webbook

rinpol	1480.05		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1729.00		NIST Webbook
tb	573.13	K	Joback Method
tc	741.92	K	Joback Method
tf	308.43	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	573.13	Joback Method
cpg	531.11	J/mol×K	601.26	Joback Method
cpg	546.77	J/mol×K	629.39	Joback Method
cpg	561.79	J/mol×K	657.52	Joback Method
cpg	576.19	J/mol×K	685.66	Joback Method
cpg	589.97	J/mol×K	713.79	Joback Method
cpg	603.14	J/mol×K	741.92	Joback Method
dvisc	0.0029408	Pa×s	308.43	Joback Method
dvisc	0.0013589	Pa×s	352.55	Joback Method
dvisc	0.0007456	Pa×s	396.66	Joback Method
dvisc	0.0004613	Pa×s	440.78	Joback Method
dvisc	0.0003115	Pa×s	484.90	Joback Method
dvisc	0.0002245	Pa×s	529.01	Joback Method
dvisc	0.0001702	Pa×s	573.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5454193&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume