4-Pentenoic acid, 2-methyl-, octyl ester

Inchi: InChI=1S/C14H26O2/c1-4-6-7-8-9-10-12-16-14(15)13(3)11-5-2/h5,13H,2,4,6-12H2,1,3H
InchiKey: SFQGNIGOIWAEBZ-UHFFFAOYSA-N
Formula: C14H26O2
SMILES: C=CCC(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-81.52	kJ/mol	Joback Method
hf	-456.94	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.102		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
tb	592.25	K	Joback Method
tc	765.51	K	Joback Method
tf	302.94	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.03	J/mol×K	592.25	Joback Method
cpg	562.74	J/mol×K	621.13	Joback Method
cpg	578.74	J/mol×K	650.00	Joback Method
cpg	594.03	J/mol×K	678.88	Joback Method
cpg	608.62	J/mol×K	707.76	Joback Method
cpg	622.55	J/mol×K	736.63	Joback Method
cpg	635.82	J/mol×K	765.51	Joback Method
dvisc	0.0035593	Pa×s	302.94	Joback Method

dvisc	0.0014576	Pa×s	351.16	Joback Method
dvisc	0.0007405	Pa×s	399.38	Joback Method
dvisc	0.0004353	Pa×s	447.60	Joback Method
dvisc	0.0002838	Pa×s	495.81	Joback Method
dvisc	0.0001995	Pa×s	544.03	Joback Method
dvisc	0.0001486	Pa×s	592.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406111&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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