

Methyl 2-hydroxydodecanoate

Inchi:	InChI=1S/C13H26O3/c1-3-4-5-6-7-8-9-10-11-12(14)13(15)16-2/h12,14H,3-11H2,1-2H3
InchiKey:	NHEBEMJQYBPWNA-UHFFFAOYSA-N
Formula:	C13H26O3
SMILES:	CCCCCCCCCCC(O)C(=O)OC
Mol. weight [g/mol]:	230.34
CAS:	51067-85-7

Physical Properties

Property code	Value	Unit	Source
gf	-314.60	kJ/mol	Joback Method
hf	-713.96	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.051		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	664.87	K	Joback Method
tc	833.68	K	Joback Method
tf	354.25	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.63	J/molxK	664.87	Joback Method
cpg	598.06	J/molxK	693.00	Joback Method
cpg	611.86	J/molxK	721.14	Joback Method
cpg	625.04	J/molxK	749.27	Joback Method
cpg	637.60	J/molxK	777.41	Joback Method

cpg	649.56	J/mol×K	805.54	Joback Method
cpg	660.93	J/mol×K	833.68	Joback Method
dvisc	0.0051687	Paxs	354.25	Joback Method
dvisc	0.0013843	Paxs	406.02	Joback Method
dvisc	0.0004994	Paxs	457.79	Joback Method
dvisc	0.0002217	Paxs	509.56	Joback Method
dvisc	0.0001143	Paxs	561.33	Joback Method
dvisc	0.0000659	Paxs	613.10	Joback Method
dvisc	0.0000414	Paxs	664.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C51067857&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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