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]: 230.35

Physical Properties

Property code	Value	Unit	Source
hf	-795.06	kJ/mol	Cheméo Relay (1.0)
hfus	32.78	kJ/mol	Joback Method
hvap	90.11	kJ/mol	Cheméo Relay (1.0)
ie	10.00	eV	Cheméo Relay (1.0)
log10ws	-3.09		Cheméo Relay (1.0)
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	545.53	K	Cheméo Relay (1.0)
tc	737.61	K	Cheméo Relay (1.0)
tf	309.71	K	Cheméo Relay (1.0)
vc	0.796	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.63	J/mol×K	664.87	Joback Method
cpg	660.93	J/mol×K	833.68	Joback Method
cpg	649.56	J/mol×K	805.54	Joback Method
cpg	637.60	J/mol×K	777.41	Joback Method
cpg	625.04	J/mol×K	749.27	Joback Method
cpg	611.86	J/mol×K	721.14	Joback Method

cpg	598.06	J/mol×K	693.00	Joback Method
dvisc	0.0002217	Pa×s	509.56	Joback Method
dvisc	0.0000414	Pa×s	664.87	Joback Method
dvisc	0.0000659	Pa×s	613.10	Joback Method
dvisc	0.0001143	Pa×s	561.33	Joback Method
dvisc	0.0051687	Pa×s	354.25	Joback Method
dvisc	0.0004994	Pa×s	457.79	Joback Method
dvisc	0.0013843	Pa×s	406.02	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51067857&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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