D-Neomenthyl-D-lactate

Inchi: InChI=1S/C13H24O3/c1-8(2)11-6-5-9(3)7-12(11)16-13(15)10(4)14/h8-12,14H,5-7H2,1-4
InchiKey: UJNOLBSYLSYIBM-VIVKNYSDSA-N
Formula: C13H24O3
SMILES: CC1CCC(C(C)C)C(OC(=O)C(C)O)C1
Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
gf	-308.01	kJ/mol	Joback Method
hf	-705.60	kJ/mol	Joback Method
hfus	23.23	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.371		Crippen Method
mcvol	196.480	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
ripol	1955.00		NIST Webbook
tb	674.64	K	Joback Method
tc	867.50	K	Joback Method
tf	338.15	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.51	J/mol×K	674.64	Joback Method
cpg	599.12	J/mol×K	706.78	Joback Method
cpg	615.74	J/mol×K	738.93	Joback Method
cpg	631.40	J/mol×K	771.07	Joback Method
cpg	646.10	J/mol×K	803.21	Joback Method
cpg	659.85	J/mol×K	835.36	Joback Method
cpg	672.66	J/mol×K	867.50	Joback Method

dvisc	0.0076841	Pa×s	338.15	Joback Method
dvisc	0.0018956	Pa×s	394.23	Joback Method
dvisc	0.0006627	Pa×s	450.31	Joback Method
dvisc	0.0002924	Pa×s	506.39	Joback Method
dvisc	0.0001519	Pa×s	562.48	Joback Method
dvisc	0.0000888	Pa×s	618.56	Joback Method
dvisc	0.0000568	Pa×s	674.64	Joback Method

Sources

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=R422723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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