Diglycolic acid, decyl neopentyl ester

Inchi: InChI=1S/C19H36O5/c1-5-6-7-8-9-10-11-12-13-23-17(20)14-22-15-18(21)24-16-19(2,3)4
InchiKey: IIWJIVFHXQNTOU-UHFFFAOYSA-N
Formula: C19H36O5
SMILES: CCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
gf	-460.90	kJ/mol	Joback Method
hf	-1066.06	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.276		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	805.89	K	Joback Method
tc	991.96	K	Joback Method
tf	472.86	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.33	J/mol×K	805.89	Joback Method
cpg	958.94	J/mol×K	836.90	Joback Method
cpg	975.48	J/mol×K	867.91	Joback Method
cpg	990.99	J/mol×K	898.92	Joback Method
cpg	1005.48	J/mol×K	929.94	Joback Method
cpg	1018.97	J/mol×K	960.95	Joback Method
cpg	1031.48	J/mol×K	991.96	Joback Method
dvisc	0.0006049	Pa×s	472.86	Joback Method

dvisc	0.0002972	Pa×s	528.37	Joback Method
dvisc	0.0001672	Pa×s	583.87	Joback Method
dvisc	0.0001039	Pa×s	639.38	Joback Method
dvisc	0.0000697	Pa×s	694.88	Joback Method
dvisc	0.0000496	Pa×s	750.38	Joback Method
dvisc	0.0000370	Pa×s	805.89	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=U381922&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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