Diglycolic acid, butyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C18H34O5/c1-5-6-11-22-17(19)13-21-14-18(20)23-12-10-16(4)9-7-8-15(2)3/h1
InchiKey: BGXNMNGUNLFJLK-UHFFFAOYSA-N
Formula: C18H34O5
SMILES: CCCCOC(=O)COCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	-477.04	kJ/mol	Joback Method
hf	-1047.23	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	75.61	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.742		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook
tb	785.36	K	Joback Method
tc	968.70	K	Joback Method
tf	429.17	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.46	J/mol×K	785.36	Joback Method
cpg	898.90	J/mol×K	815.92	Joback Method
cpg	915.32	J/mol×K	846.47	Joback Method
cpg	930.73	J/mol×K	877.03	Joback Method
cpg	945.13	J/mol×K	907.59	Joback Method
cpg	958.52	J/mol×K	938.14	Joback Method
cpg	970.92	J/mol×K	968.70	Joback Method
dvisc	0.0010058	Pa×s	429.17	Joback Method

dvisc	0.0004376	Pa×s	488.53	Joback Method
dvisc	0.0002280	Pa×s	547.90	Joback Method
dvisc	0.0001349	Pa×s	607.26	Joback Method
dvisc	0.0000877	Pa×s	666.63	Joback Method
dvisc	0.0000611	Pa×s	726.00	Joback Method
dvisc	0.0000450	Pa×s	785.36	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=U382145&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