Diglycolic acid, butyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C16H30O5/c1-6-7-8-20-14(17)11-19-12-15(18)21-10-13(2)9-16(3,4)5/h13H,6-1

InchiKey: SGWHYGMUIFVPMJ-UHFFFAOYSA-N

Formula: C16H30O5

SMILES: CCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-488.60	kJ/mol	Joback Method
hf	-1009.42	kJ/mol	Joback Method
hfus	33.02	kJ/mol	Joback Method
hvap	70.25	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.962		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook
tb	736.81	K	Joback Method
tc	921.18	K	Joback Method
tf	424.05	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.03	J/mol×K	736.81	Joback Method
cpg	840.70	J/mol×K	890.45	Joback Method
cpg	827.59	J/mol×K	859.72	Joback Method
cpg	813.57	J/mol×K	829.00	Joback Method
cpg	798.65	J/mol×K	798.27	Joback Method
cpg	782.81	J/mol×K	767.54	Joback Method
cpg	852.93	J/mol×K	921.18	Joback Method
dvisc	0.0000537	Pa×s	736.81	Joback Method

dvisc	0.0000728	Pa×s	684.68	Joback Method
dvisc	0.0001039	Pa×s	632.56	Joback Method
dvisc	0.0001580	Pa×s	580.43	Joback Method
dvisc	0.0002611	Pa×s	528.30	Joback Method
dvisc	0.0004815	Pa×s	476.18	Joback Method
dvisc	0.0010322	Pa×s	424.05	Joback Method

Sources

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=U382038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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