Diglycolic acid, butyl heptyl ester

Inchi: InChI=1S/C15H28O5/c1-3-5-7-8-9-11-20-15(17)13-18-12-14(16)19-10-6-4-2/h3-13H2,1-2
InchiKey: KREGXZUEYFINIZ-UHFFFAOYSA-N
Formula: C15H28O5
SMILES: CCCCCCCOC(=O)COCC(=O)OCCCC
Mol. weight [g/mol]: 288.38

Physical Properties

Property code	Value	Unit	Source
gf	-497.42	kJ/mol	Joback Method
hf	-974.75	kJ/mol	Joback Method
hfus	41.37	kJ/mol	Joback Method
hvap	69.71	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.860		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2395.00		NIST Webbook
tb	717.60	K	Joback Method
tc	894.31	K	Joback Method
tf	425.36	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.75	J/mol×K	717.60	Joback Method
cpg	778.49	J/mol×K	864.86	Joback Method
cpg	765.73	J/mol×K	835.41	Joback Method
cpg	752.18	J/mol×K	805.96	Joback Method
cpg	737.83	J/mol×K	776.50	Joback Method
cpg	722.68	J/mol×K	747.05	Joback Method
cpg	790.45	J/mol×K	894.31	Joback Method
dvisc	0.0000807	Pa×s	717.60	Joback Method

dvisc	0.0001048	Pa×s	668.89	Joback Method
dvisc	0.0001419	Pa×s	620.19	Joback Method
dvisc	0.0002024	Pa×s	571.48	Joback Method
dvisc	0.0003082	Pa×s	522.77	Joback Method
dvisc	0.0005119	Pa×s	474.07	Joback Method
dvisc	0.0009550	Pa×s	425.36	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=U381953&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