Diglycolic acid, butyl hexadecyl ester

Inchi: InChI=1S/C24H46O5/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-29-24(26)22-27-21-2
InchiKey: RVCAMBCQSXMFQK-UHFFFAOYSA-N
Formula: C24H46O5
SMILES: CCCCCCCCCCCCCCCCOC(=O)COCC(=O)OCCCC
Mol. weight [g/mol]: 414.62

Physical Properties

Property code	Value	Unit	Source
gf	-421.64	kJ/mol	Joback Method
hf	-1160.51	kJ/mol	Joback Method
hfus	64.68	kJ/mol	Joback Method
hvap	89.74	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.371		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	3593.00		NIST Webbook
rinpol	3593.00		NIST Webbook
tb	923.52	K	Joback Method
tc	1134.13	K	Joback Method
tf	526.79	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.72	J/mol×K	923.52	Joback Method
cpg	1269.63	J/mol×K	958.62	Joback Method
cpg	1287.94	J/mol×K	993.72	Joback Method
cpg	1304.68	J/mol×K	1028.83	Joback Method
cpg	1319.88	J/mol×K	1063.93	Joback Method
cpg	1333.55	J/mol×K	1099.03	Joback Method
cpg	1345.72	J/mol×K	1134.13	Joback Method
dvisc	0.0003557	Pa×s	526.79	Joback Method

dvisc	0.0001721	Pa×s	592.91	Joback Method
dvisc	0.0000963	Pa×s	659.03	Joback Method
dvisc	0.0000599	Pa×s	725.15	Joback Method
dvisc	0.0000404	Pa×s	791.28	Joback Method
dvisc	0.0000289	Pa×s	857.40	Joback Method
dvisc	0.0000217	Pa×s	923.52	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=U381853&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume