Diglycolic acid, butyl 4-methoxybenzyl ester

Inchi: InChI=1S/C16H22O6/c1-3-4-9-21-15(17)11-20-12-16(18)22-10-13-5-7-14(19-2)8-6-13/h5
InchiKey: CTJUMKDMFCJCIN-UHFFFAOYSA-N
Formula: C16H22O6
SMILES: CCCCOC(=O)COCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
gf	-491.22	kJ/mol	Joback Method
hf	-902.55	kJ/mol	Joback Method
hfus	38.80	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.098		Crippen Method
mcvol	239.160	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tb	794.56	K	Joback Method
tc	995.40	K	Joback Method
tf	497.80	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.14	J/mol×K	794.56	Joback Method
cpg	765.19	J/mol×K	961.93	Joback Method
cpg	755.15	J/mol×K	928.46	Joback Method
cpg	744.01	J/mol×K	894.98	Joback Method
cpg	731.79	J/mol×K	861.51	Joback Method
cpg	718.49	J/mol×K	828.03	Joback Method
cpg	774.12	J/mol×K	995.40	Joback Method
dvisc	0.0000540	Pa×s	794.56	Joback Method

dvisc	0.0000682	Pa×s	745.10	Joback Method
dvisc	0.0000889	Pa×s	695.64	Joback Method
dvisc	0.0001207	Pa×s	646.18	Joback Method
dvisc	0.0001724	Pa×s	596.72	Joback Method
dvisc	0.0002627	Pa×s	547.26	Joback Method
dvisc	0.0004351	Pa×s	497.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382248&Units=SI
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

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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