

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000682	Paxs	745.10	Joback Method
dvisc	0.0000889	Paxs	695.64	Joback Method
dvisc	0.0001207	Paxs	646.18	Joback Method
dvisc	0.0001724	Paxs	596.72	Joback Method
dvisc	0.0002627	Paxs	547.26	Joback Method
dvisc	0.0004351	Paxs	497.80	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=U382248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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