

Diglycolic acid, hexyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C17H24O6/c1-3-4-5-6-11-22-16(18)12-21-13-17(19)23-15-9-7-14(20-2)8-10-15
InchiKey:	DOTIUAQKNCBUOH-UHFFFAOYSA-N
Formula:	C17H24O6
SMILES:	CCCCCOC(=O)COCC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	324.37

Physical Properties

Property code	Value	Unit	Source
gf	-482.80	kJ/mol	Joback Method
hf	-923.19	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	79.51	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.741		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpola	2990.00		NIST Webbook
rinpola	2990.00		NIST Webbook
tb	817.44	K	Joback Method
tc	1017.95	K	Joback Method
tf	509.07	K	Joback Method
vc	0.964	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.96	J/molxK	817.44	Joback Method
cpg	775.54	J/molxK	850.86	Joback Method
cpg	789.01	J/molxK	884.28	Joback Method
cpg	801.34	J/molxK	917.70	Joback Method
cpg	812.54	J/molxK	951.12	Joback Method
cpg	822.59	J/molxK	984.53	Joback Method
cpg	831.48	J/molxK	1017.95	Joback Method
dvisc	0.0003963	Paxs	509.07	Joback Method

dvisc	0.0002361	Paxs	560.47	Joback Method
dvisc	0.0001535	Paxs	611.86	Joback Method
dvisc	0.0001067	Paxs	663.25	Joback Method
dvisc	0.0000781	Paxs	714.65	Joback Method
dvisc	0.0000596	Paxs	766.04	Joback Method
dvisc	0.0000471	Paxs	817.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381887&Units=SI

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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