

Diglycolic acid, 2-methoxyphenyl propyl ester

Inchi: InChI=1S/C14H18O6/c1-3-8-19-13(15)9-18-10-14(16)20-12-7-5-4-6-11(12)17-2/h4-7H,3,
InchiKey: AYSQXAPEPBNMH-UHFFFAOYSA-N
Formula: C14H18O6
SMILES: CCCOC(=O)COCC(=O)Oc1ccccc1OC
Mol. weight [g/mol]: 282.29

Physical Properties

Property code	Value	Unit	Source
gf	-508.06	kJ/mol	Joback Method
hf	-861.27	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	72.83	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.570		Crippen Method
mcvol	210.980	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpola	2532.00		NIST Webbook
rinpola	2532.00		NIST Webbook
tb	748.80	K	Joback Method
tc	952.07	K	Joback Method
tf	475.26	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.40	J/molxK	748.80	Joback Method
cpg	607.15	J/molxK	782.68	Joback Method
cpg	619.95	J/molxK	816.56	Joback Method
cpg	631.79	J/molxK	850.44	Joback Method
cpg	642.65	J/molxK	884.31	Joback Method
cpg	652.51	J/molxK	918.19	Joback Method
cpg	661.35	J/molxK	952.07	Joback Method
dvisc	0.0005167	Paxs	475.26	Joback Method

dvisc	0.0003206	Paxs	520.85	Joback Method
dvisc	0.0002148	Paxs	566.44	Joback Method
dvisc	0.0001528	Paxs	612.03	Joback Method
dvisc	0.0001139	Paxs	657.62	Joback Method
dvisc	0.0000882	Paxs	703.21	Joback Method
dvisc	0.0000705	Paxs	748.80	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=U382240&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

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