

Diglycolic acid, hexyl 2-isopropylphenyl ester

Inchi:	InChI=1S/C19H28O5/c1-4-5-6-9-12-23-18(20)13-22-14-19(21)24-17-11-8-7-10-16(17)15
InchiKey:	HVSOYJQRJDLWKT-UHFFFAOYSA-N
Formula:	C19H28O5
SMILES:	CCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]:	336.42

Physical Properties

Property code	Value	Unit	Source
gf	-363.40	kJ/mol	Joback Method
hf	-837.53	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	81.16	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.856		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinqol	2821.00		NIST Webbook
tb	840.34	K	Joback Method
tc	1042.54	K	Joback Method
tf	494.38	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.69	J/molxK	840.34	Joback Method
cpg	914.81	J/molxK	1008.84	Joback Method
cpg	903.93	J/molxK	975.14	Joback Method
cpg	891.88	J/molxK	941.44	Joback Method
cpg	878.66	J/molxK	907.74	Joback Method
cpg	864.27	J/molxK	874.04	Joback Method
cpg	924.54	J/molxK	1042.54	Joback Method
dvisc	0.0000434	Paxs	840.34	Joback Method
dvisc	0.0000564	Paxs	782.68	Joback Method

dvisc	0.0000763	Paxs	725.02	Joback Method
dvisc	0.0001088	Paxs	667.36	Joback Method
dvisc	0.0001659	Paxs	609.70	Joback Method
dvisc	0.0002763	Paxs	552.04	Joback Method
dvisc	0.0005184	Paxs	494.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382291&Units=SI
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

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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