

Diglycolic acid, heptyl 3-phenylpropyl ester

Inchi:	InChI=1S/C20H30O5/c1-2-3-4-5-9-14-24-19(21)16-23-17-20(22)25-15-10-13-18-11-7-6-8
InchiKey:	XGNQEJFTCLKEPA-UHFFFAOYSA-N
Formula:	C20H30O5
SMILES:	CCCCCCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	350.45

Physical Properties

Property code	Value	Unit	Source
gf	-342.91	kJ/mol	Joback Method
hf	-841.42	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	83.11	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.693		Crippen Method
mvol	289.650	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	3274.00		NIST Webbook
rinpol	3274.00		NIST Webbook
tb	858.68	K	Joback Method
tc	1059.32	K	Joback Method
tf	508.13	K	Joback Method
vc	1.113	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.79	J/molxK	858.68	Joback Method
cpg	923.53	J/molxK	892.12	Joback Method
cpg	938.06	J/molxK	925.56	Joback Method
cpg	951.40	J/molxK	959.00	Joback Method
cpg	963.57	J/molxK	992.44	Joback Method
cpg	974.58	J/molxK	1025.88	Joback Method
cpg	984.46	J/molxK	1059.32	Joback Method
dvisc	0.0004837	Paxs	508.13	Joback Method

dvisc	0.0002586	Paxs	566.55	Joback Method
dvisc	0.0001554	Paxs	624.98	Joback Method
dvisc	0.0001019	Paxs	683.40	Joback Method
dvisc	0.0000714	Paxs	741.83	Joback Method
dvisc	0.0000527	Paxs	800.25	Joback Method
dvisc	0.0000405	Paxs	858.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382176&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
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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