

Diglycolic acid, heptyl 2-isopropylphenyl ester

Inchi:	InChI=1S/C20H30O5/c1-4-5-6-7-10-13-24-19(21)14-23-15-20(22)25-18-12-9-8-11-17(18)
InchiKey:	PPSGSKFSSIRVSS-UHFFFAOYSA-N
Formula:	C20H30O5
SMILES:	CCCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]:	350.45

Physical Properties

Property code	Value	Unit	Source
gf	-354.98	kJ/mol	Joback Method
hf	-858.17	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	83.39	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.246		Crippen Method
mvol	289.650	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2950.00		NIST Webbook
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tb	863.22	K	Joback Method
tc	1066.21	K	Joback Method
tf	505.65	K	Joback Method
vc	1.107	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.61	J/molxK	863.22	Joback Method
cpg	923.35	J/molxK	897.05	Joback Method
cpg	937.85	J/molxK	930.88	Joback Method
cpg	951.12	J/molxK	964.72	Joback Method
cpg	963.17	J/molxK	998.55	Joback Method
cpg	974.01	J/molxK	1032.38	Joback Method
cpg	983.65	J/molxK	1066.21	Joback Method
dvisc	0.0004662	Paxs	505.65	Joback Method

dvisc	0.0002457	Paxs	565.25	Joback Method
dvisc	0.0001463	Paxs	624.84	Joback Method
dvisc	0.0000953	Paxs	684.43	Joback Method
dvisc	0.0000666	Paxs	744.03	Joback Method
dvisc	0.0000490	Paxs	803.62	Joback Method
dvisc	0.0000376	Paxs	863.22	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=U382292&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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