

Diglycolic acid, isohexyl 2-naphthyl ester

Inchi:	InChI=1S/C20H24O5/c1-15(2)6-5-11-24-19(21)13-23-14-20(22)25-18-10-9-16-7-3-4-8-17
InchiKey:	JXZCTQNGFAHKPH-UHFFFAOYSA-N
Formula:	C20H24O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	344.40

Physical Properties

Property code	Value	Unit	Source
gf	-248.33	kJ/mol	Joback Method
hf	-667.10	kJ/mol	Joback Method
hfus	41.47	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.741		Crippen Method
mcvol	270.190	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinsol	3336.00		NIST Webbook
tb	882.20	K	Joback Method
tc	1098.37	K	Joback Method
tf	538.35	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.15	J/molxK	882.20	Joback Method
cpg	890.15	J/molxK	1062.34	Joback Method
cpg	880.56	J/molxK	1026.32	Joback Method
cpg	869.89	J/molxK	990.29	Joback Method
cpg	858.13	J/molxK	954.26	Joback Method
cpg	845.23	J/molxK	918.23	Joback Method
cpg	898.71	J/molxK	1098.37	Joback Method
dvisc	0.0000751	Paxs	882.20	Joback Method
dvisc	0.0000934	Paxs	824.89	Joback Method

dvisc	0.0001201	Paxs	767.58	Joback Method
dvisc	0.0001608	Paxs	710.28	Joback Method
dvisc	0.0002265	Paxs	652.97	Joback Method
dvisc	0.0003409	Paxs	595.66	Joback Method
dvisc	0.0005597	Paxs	538.35	Joback Method

Sources

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=U381789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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