

Glutaric acid, 3-methylbut-2-yl 2,4-dichloro-1-naphthyl ester

Inchi:	InChI=1S/C20H22Cl2O4/c1-12(2)13(3)25-18(23)9-6-10-19(24)26-20-15-8-5-4-7-14(15)16
InchiKey:	HBRAOYDFYWGWR-UHFFFAOYSA-N
Formula:	C20H22Cl2O4
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]:	397.29

Physical Properties

Property code	Value	Unit	Source
gf	-188.89	kJ/mol	Joback Method
hf	-594.58	kJ/mol	Joback Method
hfus	44.37	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.810		Crippen Method
mvol	288.800	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2859.00		NIST Webbook
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tb	944.16	K	Joback Method
tc	1172.54	K	Joback Method
tf	586.00	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.86	J/molxK	944.16	Joback Method
cpg	860.06	J/molxK	982.22	Joback Method
cpg	871.15	J/molxK	1020.29	Joback Method
cpg	881.18	J/molxK	1058.35	Joback Method
cpg	890.20	J/molxK	1096.41	Joback Method
cpg	898.25	J/molxK	1134.47	Joback Method
cpg	905.40	J/molxK	1172.54	Joback Method
dvisc	0.0004778	Paxs	586.00	Joback Method

dvisc	0.0003009	Paxs	645.69	Joback Method
dvisc	0.0002049	Paxs	705.39	Joback Method
dvisc	0.0001482	Paxs	765.08	Joback Method
dvisc	0.0001123	Paxs	824.77	Joback Method
dvisc	0.0000884	Paxs	884.47	Joback Method
dvisc	0.0000717	Paxs	944.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392017&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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