

Glutaric acid, hept-2-yl 2,4-dichloro-1-naphthyl ester

Inchi:	InChI=1S/C22H26Cl2O4/c1-3-4-5-9-15(2)27-20(25)12-8-13-21(26)28-22-17-11-7-6-10-16
InchiKey:	RIQAWQRLNWKFHN-UHFFFAOYSA-N
Formula:	C22H26Cl2O4
SMILES:	CCCCC(C)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]:	425.35

Physical Properties

Property code	Value	Unit	Source
gf	-169.61	kJ/mol	Joback Method
hf	-630.58	kJ/mol	Joback Method
hfus	53.07	kJ/mol	Joback Method
hvap	97.16	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	6.734		Crippen Method
mcvol	316.980	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	990.36	K	Joback Method
tc	1218.30	K	Joback Method
tf	623.54	K	Joback Method
vc	1.222	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.72	J/molxK	990.36	Joback Method
cpg	1016.73	J/molxK	1180.31	Joback Method
cpg	1008.37	J/molxK	1142.32	Joback Method
cpg	999.04	J/molxK	1104.33	Joback Method
cpg	988.70	J/molxK	1066.34	Joback Method
cpg	977.28	J/molxK	1028.35	Joback Method
cpg	1024.18	J/molxK	1218.30	Joback Method
dvisc	0.0000594	Paxs	990.36	Joback Method

dvisc	0.0000728	Paxs	929.22	Joback Method
dvisc	0.0000920	Paxs	868.09	Joback Method
dvisc	0.0001204	Paxs	806.95	Joback Method
dvisc	0.0001646	Paxs	745.81	Joback Method
dvisc	0.0002380	Paxs	684.68	Joback Method
dvisc	0.0003701	Paxs	623.54	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=U392022&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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