

Glutaric acid, 2,4-dichloronaphthyl octyl ester

Inchi:	InChI=1S/C23H28Cl2O4/c1-2-3-4-5-6-9-15-28-21(26)13-10-14-22(27)29-23-18-12-8-7-1
InchiKey:	LIVUMWCFPYRRLG-UHFFFAOYSA-N
Formula:	C23H28Cl2O4
SMILES:	CCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2cccc12
Mol. weight [g/mol]:	439.37

Physical Properties

Property code	Value	Unit	Source
gf	-158.75	kJ/mol	Joback Method
hf	-645.94	kJ/mol	Joback Method
hfus	59.19	kJ/mol	Joback Method
hvap	99.78	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.126		Crippen Method
mvol	331.070	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	3333.00		NIST Webbook
rinpol	3333.00		NIST Webbook
tb	1013.68	K	Joback Method
tc	1243.03	K	Joback Method
tf	649.81	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.94	J/molxK	1013.68	Joback Method
cpg	1036.74	J/molxK	1051.91	Joback Method
cpg	1048.40	J/molxK	1090.13	Joback Method
cpg	1058.97	J/molxK	1128.36	Joback Method
cpg	1068.51	J/molxK	1166.58	Joback Method
cpg	1077.10	J/molxK	1204.81	Joback Method
cpg	1084.78	J/molxK	1243.03	Joback Method
dvisc	0.0003199	Paxs	649.81	Joback Method

dvisc	0.0002119	Paxs	710.46	Joback Method
dvisc	0.0001497	Paxs	771.10	Joback Method
dvisc	0.0001113	Paxs	831.75	Joback Method
dvisc	0.0000861	Paxs	892.39	Joback Method
dvisc	0.0000688	Paxs	953.04	Joback Method
dvisc	0.0000565	Paxs	1013.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358928&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

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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