

Glutaric acid, 2,6-dichlorophenyl hexadecyl ester

Inchi:	InChI=1S/C27H42Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-32-25(30)20-17-21-2
InchiKey:	BTLSWUMMEKLBKP-UHFFFAOYSA-N
Formula:	C27H42Cl2O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	501.53

Physical Properties

Property code	Value	Unit	Source
gf	-222.09	kJ/mol	Joback Method
hf	-908.10	kJ/mol	Joback Method
hfus	72.92	kJ/mol	Joback Method
hvap	106.38	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	9.094		Crippen Method
mcvol	406.890	ml/mol	McGowan Method
pc	820.54	kPa	Joback Method
rinpol	3622.00		NIST Webbook
rinpol	3622.00		NIST Webbook
tb	1081.24	K	Joback Method
tc	1331.71	K	Joback Method
tf	649.67	K	Joback Method
vc	1.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.70	J/molxK	1081.24	Joback Method
cpg	1413.69	J/molxK	1289.96	Joback Method
cpg	1405.28	J/molxK	1248.22	Joback Method
cpg	1395.25	J/molxK	1206.47	Joback Method
cpg	1383.53	J/molxK	1164.73	Joback Method
cpg	1370.04	J/molxK	1122.98	Joback Method
cpg	1420.56	J/molxK	1331.71	Joback Method
dvisc	0.0000139	Paxs	1081.24	Joback Method

dvisc	0.0000179	Paxs	1009.31	Joback Method
dvisc	0.0000241	Paxs	937.38	Joback Method
dvisc	0.0000339	Paxs	865.45	Joback Method
dvisc	0.0000508	Paxs	793.53	Joback Method
dvisc	0.0000825	Paxs	721.60	Joback Method
dvisc	0.0001493	Paxs	649.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358843&Units=SI

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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