

Glutaric acid, dodec-2-en-1-yl 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C23H32Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-18-28-21(26)16-13-17-22(27)29-20-15
InchiKey:	LHLPXHURRXKTRC-ZHACJKMWSA-N
Formula:	C23H32Cl2O4
SMILES:	CCCCCCCCC=CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	443.40

Physical Properties

Property code	Value	Unit	Source
gf	-175.55	kJ/mol	Joback Method
hf	-708.32	kJ/mol	Joback Method
hfus	62.76	kJ/mol	Joback Method
hvap	97.43	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	7.309		Crippen Method
mcvol	346.230	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpola	3153.00		NIST Webbook
rinpola	3153.00		NIST Webbook
tb	993.88	K	Joback Method
tc	1217.25	K	Joback Method
tf	599.51	K	Joback Method
vc	1.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.91	J/molxK	993.88	Joback Method
cpg	1138.66	J/molxK	1180.03	Joback Method
cpg	1129.16	J/molxK	1142.80	Joback Method
cpg	1118.59	J/molxK	1105.57	Joback Method
cpg	1106.89	J/molxK	1068.34	Joback Method
cpg	1094.02	J/molxK	1031.11	Joback Method
cpg	1147.14	J/molxK	1217.25	Joback Method
dvisc	0.0000229	Paxs	993.88	Joback Method

dvisc	0.0000293	Paxs	928.15	Joback Method
dvisc	0.0000389	Paxs	862.42	Joback Method
dvisc	0.0000542	Paxs	796.69	Joback Method
dvisc	0.0000801	Paxs	730.97	Joback Method
dvisc	0.0001280	Paxs	665.24	Joback Method
dvisc	0.0002264	Paxs	599.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391994&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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