

Glutaric acid, 2-norbornyl 3-chlorophenyl ester

Inchi:	InChI=1S/C18H21ClO4/c19-14-3-1-4-15(11-14)22-17(20)5-2-6-18(21)23-16-10-12-7-8-13
InchiKey:	NREYGRFFRGHUOG-UHFFFAOYSA-N
Formula:	C18H21ClO4
SMILES:	O=C(CCCC(=O)OC1CC2CCC1C2)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	336.81

Physical Properties

Property code	Value	Unit	Source
gf	-174.62	kJ/mol	Joback Method
hf	-576.03	kJ/mol	Joback Method
hfus	41.04	kJ/mol	Joback Method
hvap	80.99	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.147		Crippen Method
mcvol	246.120	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		NIST Webbook
tb	845.99	K	Joback Method
tc	1072.66	K	Joback Method
tf	533.92	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.93	J/molxK	845.99	Joback Method
cpg	827.80	J/molxK	1034.88	Joback Method
cpg	816.74	J/molxK	997.10	Joback Method
cpg	804.70	J/molxK	959.33	Joback Method
cpg	791.60	J/molxK	921.55	Joback Method
cpg	777.37	J/molxK	883.77	Joback Method
cpg	837.95	J/molxK	1072.66	Joback Method
dvisc	0.0005388	Paxs	845.99	Joback Method

dvisc	0.0006208	Paxs	793.98	Joback Method
dvisc	0.0007297	Paxs	741.97	Joback Method
dvisc	0.0008787	Paxs	689.96	Joback Method
dvisc	0.0010908	Paxs	637.94	Joback Method
dvisc	0.0014070	Paxs	585.93	Joback Method
dvisc	0.0019071	Paxs	533.92	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=U405496&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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