

Glutaric acid, 3-chlorophenyl 2,4-dichlorophenyl ester

Inchi:	InChI=1S/C17H13Cl3O4/c18-11-3-1-4-13(9-11)23-16(21)5-2-6-17(22)24-15-8-7-12(19)10
InchiKey:	GSKAHLWCFJCOEJ-UHFFFAOYSA-N
Formula:	C17H13Cl3O4
SMILES:	O=C(CCCC(=O)Oc1ccc(Cl)cc1Cl)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	387.64

Physical Properties

Property code	Value	Unit	Source
gf	-215.44	kJ/mol	Joback Method
hf	-492.38	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	91.44	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.328		Crippen Method
mcvol	254.470	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2846.00		NIST Webbook
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tb	921.53	K	Joback Method
tc	1162.77	K	Joback Method
tf	605.83	K	Joback Method
vc	0.967	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.67	J/mol×K	921.53	Joback Method
cpg	682.15	J/mol×K	961.74	Joback Method
cpg	690.43	J/mol×K	1001.94	Joback Method
cpg	697.53	J/mol×K	1042.15	Joback Method
cpg	703.48	J/mol×K	1082.35	Joback Method
cpg	708.30	J/mol×K	1122.56	Joback Method
cpg	712.03	J/mol×K	1162.77	Joback Method
dvisc	0.0003250	Paxs	605.83	Joback Method

dvisc	0.0002167	Paxs	658.45	Joback Method
dvisc	0.0001534	Paxs	711.06	Joback Method
dvisc	0.0001138	Paxs	763.68	Joback Method
dvisc	0.0000878	Paxs	816.30	Joback Method
dvisc	0.0000699	Paxs	868.91	Joback Method
dvisc	0.0000571	Paxs	921.53	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=U391857&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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