

Glutaric acid, 3-chlorobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C19H27ClO4/c1-4-7-17(14(2)3)24-19(22)11-6-10-18(21)23-13-15-8-5-9-16(20)
InchiKey:	KIH XOAVGPRMQLG-UHFFFAOYSA-N
Formula:	C19H27ClO4
SMILES:	CCCC(OC(=O)CCCC(=O)OCc1cccc(Cl)c1)C(C)C
Mol. weight [g/mol]:	354.87

Physical Properties

Property code	Value	Unit	Source
gf	-272.77	kJ/mol	Joback Method
hf	-726.33	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.921		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2647.00		NIST Webbook
tb	854.91	K	Joback Method
tc	1063.12	K	Joback Method
tf	487.07	K	Joback Method
vc	1.077	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.35	J/molxK	854.91	Joback Method
cpg	862.34	J/molxK	889.61	Joback Method
cpg	876.17	J/molxK	924.31	Joback Method
cpg	888.84	J/molxK	959.02	Joback Method
cpg	900.40	J/molxK	993.72	Joback Method
cpg	910.86	J/molxK	1028.42	Joback Method
cpg	920.25	J/molxK	1063.12	Joback Method
dvisc	0.0006863	Paxs	487.07	Joback Method
dvisc	0.0003396	Paxs	548.38	Joback Method

dvisc	0.0001936	Paxs	609.68	Joback Method
dvisc	0.0001223	Paxs	670.99	Joback Method
dvisc	0.0000834	Paxs	732.30	Joback Method
dvisc	0.0000604	Paxs	793.60	Joback Method
dvisc	0.0000458	Paxs	854.91	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=U377593&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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