

Glutaric acid, (2-chlorocyclohexyl)methyl 8-chlorooctyl ester

Inchi:	InChI=1S/C20H34Cl2O4/c21-14-7-3-1-2-4-8-15-25-19(23)12-9-13-20(24)26-16-17-10-5-6
InchiKey:	KRGSMTNTYJUOOJ-UHFFFAOYSA-N
Formula:	C20H34Cl2O4
SMILES:	O=C(CCCC(=O)OCC1CCCCC1Cl)OCCCCCCCCCl
Mol. weight [g/mol]:	409.39

Physical Properties

Property code	Value	Unit	Source
gf	-357.44	kJ/mol	Joback Method
hf	-943.23	kJ/mol	Joback Method
hfus	54.43	kJ/mol	Joback Method
hvap	87.32	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.620		Crippen Method
mvol	321.160	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	3035.00		NIST Webbook
rinpol	3035.00		NIST Webbook
tb	899.32	K	Joback Method
tc	1106.01	K	Joback Method
tf	522.46	K	Joback Method
vc	1.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.89	J/molxK	899.32	Joback Method
cpg	1099.01	J/molxK	1071.56	Joback Method
cpg	1087.92	J/molxK	1037.11	Joback Method
cpg	1075.48	J/molxK	1002.66	Joback Method
cpg	1061.68	J/molxK	968.22	Joback Method
cpg	1046.49	J/molxK	933.77	Joback Method
cpg	1108.79	J/molxK	1106.01	Joback Method
dvisc	0.0000520	Paxs	899.32	Joback Method

dvisc	0.0000677	Paxs	836.51	Joback Method
dvisc	0.0000919	Paxs	773.70	Joback Method
dvisc	0.0001317	Paxs	710.89	Joback Method
dvisc	0.0002023	Paxs	648.08	Joback Method
dvisc	0.0003408	Paxs	585.27	Joback Method
dvisc	0.0006508	Paxs	522.46	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=U405452&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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