

Glutaric acid, (cyclohex-3-enyl)methyl 8-chlorooctyl ester

Inchi:	InChI=1S/C20H33ClO4/c21-15-8-3-1-2-4-9-16-24-19(22)13-10-14-20(23)25-17-18-11-6-5
InchiKey:	UUJAQSUDWFRZOV-UHFFFAOYSA-N
Formula:	C20H33ClO4
SMILES:	O=C(CCCC(=O)OCC1CC=CCC1)OCCCCCCCCCl
Mol. weight [g/mol]:	372.93

Physical Properties

Property code	Value	Unit	Source
gf	-307.84	kJ/mol	Joback Method
hf	-849.37	kJ/mol	Joback Method
hfus	50.38	kJ/mol	Joback Method
hvap	83.53	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.179		Crippen Method
mvol	304.620	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	2808.00		NIST Webbook
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tb	865.72	K	Joback Method
tc	1067.63	K	Joback Method
tf	497.54	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.32	J/molxK	865.72	Joback Method
cpg	1040.31	J/molxK	1033.98	Joback Method
cpg	1028.35	J/molxK	1000.33	Joback Method
cpg	1015.21	J/molxK	966.68	Joback Method
cpg	1000.84	J/molxK	933.02	Joback Method
cpg	985.22	J/molxK	899.37	Joback Method
cpg	1051.09	J/molxK	1067.63	Joback Method
dvisc	0.0000509	Paxs	865.72	Joback Method

dvisc	0.0000670	Paxs	804.36	Joback Method
dvisc	0.0000924	Paxs	742.99	Joback Method
dvisc	0.0001351	Paxs	681.63	Joback Method
dvisc	0.0002128	Paxs	620.27	Joback Method
dvisc	0.0003703	Paxs	558.90	Joback Method
dvisc	0.0007387	Paxs	497.54	Joback Method

Sources

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=U405533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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