

Glutaric acid, cyclopentyl 8-chlorooctyl ester

Inchi:	InChI=1S/C18H31ClO4/c19-14-7-3-1-2-4-8-15-22-17(20)12-9-13-18(21)23-16-10-5-6-11
InchiKey:	FDKTUNPKOMZURW-UHFFFAOYSA-N
Formula:	C18H31ClO4
SMILES:	O=C(CCCC(=O)OC1CCCC1)OCCCCCCCCCl
Mol. weight [g/mol]:	346.89

Physical Properties

Property code	Value	Unit	Source
gf	-342.54	kJ/mol	Joback Method
hf	-859.71	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	78.62	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.765		Crippen Method
mvol	280.740	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	816.53	K	Joback Method
tc	1012.64	K	Joback Method
tf	477.76	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.00	J/molxK	816.53	Joback Method
cpg	890.07	J/molxK	849.21	Joback Method
cpg	906.00	J/molxK	881.90	Joback Method
cpg	920.83	J/molxK	914.58	Joback Method
cpg	934.58	J/molxK	947.27	Joback Method
cpg	947.29	J/molxK	979.95	Joback Method
cpg	958.97	J/molxK	1012.64	Joback Method
dvisc	0.0010512	Paxs	477.76	Joback Method

dvisc	0.0005628	Paxs	534.22	Joback Method
dvisc	0.0003395	Paxs	590.68	Joback Method
dvisc	0.0002237	Paxs	647.14	Joback Method
dvisc	0.0001576	Paxs	703.61	Joback Method
dvisc	0.0001170	Paxs	760.07	Joback Method
dvisc	0.0000905	Paxs	816.53	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=U405400&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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