Glutaric acid, 8-chlorooctyl 3-methylbutyl ester

Inchi: InChI=1S/C18H33ClO4/c1-16(2)12-15-23-18(21)11-9-10-17(20)22-14-8-6-4-3-5-7-13-19/

InchiKey: RJHFTJOIMWHTJU-UHFFFAOYSA-N

Formula: C18H33ClO4

SMILES: CC(C)CCOC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 348.90

Physical Properties

Property code	Value	Unit	Source
gf	-381.53	kJ/mol	Joback Method
hf	-925.47	kJ/mol	Joback Method
hfus	48.62	kJ/mol	Joback Method
hvap	77.97	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.869		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tb	800.81	K	Joback Method
tc	986.70	K	Joback Method
tf	451.86	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.59	J/mol×K	800.81	Joback Method
cpg	955.10	J/mol×K	955.71	Joback Method
cpg	942.30	J/mol×K	924.73	Joback Method
cpg	928.56	J/mol×K	893.75	Joback Method
cpg	913.87	J/mol×K	862.77	Joback Method
cpg	898.22	J/mol×K	831.79	Joback Method
cpg	966.99	J/mol×K	986.70	Joback Method
dvisc	0.0000562	Pa×s	800.81	Joback Method

dvisc	0.0000750	Pa×s	742.65	Joback Method
dvisc	0.0001052	Pa×s	684.49	Joback Method
dvisc	0.0001569	Pa×s	626.34	Joback Method
dvisc	0.0002542	Pa×s	568.18	Joback Method
dvisc	0.0004596	Pa×s	510.02	Joback Method
dvisc	0.0009679	Pa×s	451.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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