Glutaric acid, 8-chlorooctyl 2-methylpentyl ester

Inchi: InChI=1S/C19H35ClO4/c1-3-11-17(2)16-24-19(22)13-10-12-18(21)23-15-9-7-5-4-6-8-14-

InchiKey: SJVGJQKWBQZNKC-UHFFFAOYSA-N

Formula: C19H35ClO4

SMILES: CCCC(C)COC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 362.93

Physical Properties

Property code	Value	Unit	Source
gf	-373.11	kJ/mol	Joback Method
hf	-946.11	kJ/mol	Joback Method
hfus	51.21	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	5.259		Crippen Method
mcvol	305.690	ml/mol	McGowan Method
pc	1126.83	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	823.69	K	Joback Method
tc	1011.93	K	Joback Method
tf	463.13	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.05	J/mol×K	823.69	Joback Method
cpg	1015.87	J/mol×K	980.56	Joback Method
cpg	1002.91	J/mol×K	949.19	Joback Method
cpg	988.97	J/mol×K	917.81	Joback Method
cpg	974.02	J/mol×K	886.44	Joback Method
cpg	958.06	J/mol×K	855.06	Joback Method
cpg	1027.85	J/mol×K	1011.93	Joback Method
dvisc	0.0000485	Pa×s	823.69	Joback Method

dvisc	0.0000649	Pa×s	763.60	Joback Method
dvisc	0.0000912	Pa×s	703.50	Joback Method
dvisc	0.0001367	Pa×s	643.41	Joback Method
dvisc	0.0002226	Pa×s	583.32	Joback Method
dvisc	0.0004054	Pa×s	523.22	Joback Method
dvisc	0.0008626	Pa×s	463.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391715&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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