Glutaric acid, 3-methylbut-2-yl 8-chlorooctyl ester

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

InchiKey: QXMMPSGXYJYUHL-UHFFFAOYSA-N

Formula: C18H33ClO4

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

Mol. weight [g/mol]: 348.90

Physical Properties

Property code	Value	Unit	Source
gf	-383.97	kJ/mol	Joback Method
hf	-930.75	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	77.58	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.867		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	800.37	K	Joback Method
tc	987.50	K	Joback Method
tf	436.86	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.09	J/mol×K	800.37	Joback Method
cpg	898.84	J/mol×K	831.56	Joback Method
cpg	914.58	J/mol×K	862.75	Joback Method
cpg	929.34	J/mol×K	893.93	Joback Method
cpg	943.13	J/mol×K	925.12	Joback Method
cpg	955.96	J/mol×K	956.31	Joback Method
cpg	967.85	J/mol×K	987.50	Joback Method
dvisc	0.0011551	Pa×s	436.86	Joback Method

dvisc	0.0005021	Pa×s	497.44	Joback Method
dvisc	0.0002615	Pa×s	558.03	Joback Method
dvisc	0.0001548	Pa×s	618.62	Joback Method
dvisc	0.0001006	Pa×s	679.20	Joback Method
dvisc	0.0000701	Pa×s	739.79	Joback Method
dvisc	0.0000517	Pa×s	800.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393459&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