Glutaric acid, oct-1-en-3-yl 8-chlorooctyl ester

Inchi: InChI=1S/C21H37ClO4/c1-3-5-10-14-19(4-2)26-21(24)16-13-15-20(23)25-18-12-9-7-6-8-
InchiKey: ODKUMRUKSOCIOC-UHFFFAOYSA-N
Formula: C21H37ClO4
SMILES: C=CC(CCCCC)OC(=O)CCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 388.97

Physical Properties

Property code	Value	Unit	Source
gf	-268.43	kJ/mol	Joback Method
hf	-861.96	kJ/mol	Joback Method
hfus	55.11	kJ/mol	Joback Method
hvap	83.98	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.957		Crippen Method
mcvol	329.570	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	2631.00		NIST Webbook
rinpol	2631.00		NIST Webbook
tb	866.13	K	Joback Method
tc	1061.15	K	Joback Method
tf	483.91	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.19	J/mol×K	866.13	Joback Method
cpg	1109.37	J/mol×K	1028.64	Joback Method
cpg	1096.49	J/mol×K	996.14	Joback Method
cpg	1082.56	J/mol×K	963.64	Joback Method
cpg	1067.55	J/mol×K	931.14	Joback Method
cpg	1051.44	J/mol×K	898.63	Joback Method
cpg	1121.23	J/mol×K	1061.15	Joback Method
dvisc	0.0000385	Pa×s	866.13	Joback Method

dvisc	0.0000515	Pa×s	802.43	Joback Method
dvisc	0.0000724	Pa×s	738.72	Joback Method
dvisc	0.0001085	Pa×s	675.02	Joback Method
dvisc	0.0001769	Pa×s	611.32	Joback Method
dvisc	0.0003234	Pa×s	547.61	Joback Method
dvisc	0.0006926	Pa×s	483.91	Joback Method

Sources

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=U405356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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