Glutaric acid, hept-2-yl 10-chlorodecyl ester

Inchi: InChI=1S/C22H41ClO4/c1-3-4-11-15-20(2)27-22(25)17-14-16-21(24)26-19-13-10-8-6-5-7
InchiKey: XYZGRCMHSGOTPH-UHFFFAOYSA-N
Formula: C22H41ClO4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCCCCCCCCCCCCl
Mol. weight [g/mol]: 405.01

Physical Properties

Property code	Value	Unit	Source
gf	-347.85	kJ/mol	Joback Method
hf	-1008.03	kJ/mol	Joback Method
hfus	58.98	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.572		Crippen Method
mcvol	347.960	ml/mol	McGowan Method
pc	936.92	kPa	Joback Method
rinpol	2761.00		NIST Webbook
rinpol	2761.00		NIST Webbook
tb	892.33	K	Joback Method
tc	1092.48	K	Joback Method
tf	496.94	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.91	J/mol×K	892.33	Joback Method
cpg	1142.13	J/mol×K	925.69	Joback Method
cpg	1159.07	J/mol×K	959.05	Joback Method
cpg	1174.77	J/mol×K	992.40	Joback Method
cpg	1189.26	J/mol×K	1025.76	Joback Method
cpg	1202.56	J/mol×K	1059.12	Joback Method
cpg	1214.70	J/mol×K	1092.48	Joback Method
dvisc	0.0005981	Pa×s	496.94	Joback Method

dvisc	0.0002731	Pa×s	562.84	Joback Method
dvisc	0.0001469	Pa×s	628.74	Joback Method
dvisc	0.0000889	Pa×s	694.63	Joback Method
dvisc	0.0000587	Pa×s	760.53	Joback Method
dvisc	0.0000414	Pa×s	826.43	Joback Method
dvisc	0.0000308	Pa×s	892.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392459&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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