Glutaric acid, di(8-chlorooctyl) ester

Inchi: InChI=1S/C21H38Cl2O4/c22-16-9-5-1-3-7-11-18-26-20(24)14-13-15-21(25)27-19-12-8-4-2-6-10-17-23
InchiKey: YMTYKVSZHOIKLD-UHFFFAOYSA-N
Formula: C21H38Cl2O4
SMILES: O=C(CCCC(=O)OCCCCCCCCCCl)OCCCCCCCCCCl
Mol. weight [g/mol]: 425.43

Physical Properties

Property code	Value	Unit	Source
gf	-365.76	kJ/mol	Joback Method
hf	-997.85	kJ/mol	Joback Method
hfus	64.11	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.402		Crippen Method
mcvol	346.110	ml/mol	McGowan Method
pc	966.87	kPa	Joback Method
rinpol	3197.00		NIST Webbook
rinpol	3197.00		NIST Webbook
tb	907.32	K	Joback Method
tc	1110.88	K	Joback Method
tf	530.59	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.16	J/mol×K	907.32	Joback Method
cpg	1163.44	J/mol×K	1076.96	Joback Method
cpg	1151.33	J/mol×K	1043.03	Joback Method
cpg	1138.07	J/mol×K	1009.10	Joback Method
cpg	1123.65	J/mol×K	975.17	Joback Method
cpg	1108.02	J/mol×K	941.25	Joback Method
cpg	1174.43	J/mol×K	1110.88	Joback Method
dvisc	0.0000330	Pa×s	907.32	Joback Method

dvisc	0.0000435	Pa×s	844.53	Joback Method
dvisc	0.0000599	Pa×s	781.74	Joback Method
dvisc	0.0000873	Pa×s	718.95	Joback Method
dvisc	0.0001366	Pa×s	656.17	Joback Method
dvisc	0.0002351	Pa×s	593.38	Joback Method
dvisc	0.0004601	Pa×s	530.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359597&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