Glutaric acid, cyclohexylmethyl 8-chlorooctyl ester

Inchi: InChI=1S/C20H35ClO4/c21-15-8-3-1-2-4-9-16-24-19(22)13-10-14-20(23)25-17-18-11-6-5

InchiKey: IFFARWVALOVMMD-UHFFFAOYSA-N

Formula: C20H35ClO4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCCCCCCCCCl

Mol. weight [g/mol]: 374.94

Physical Properties

Property code	Value	Unit	Source
gf	-337.80	kJ/mol	Joback Method
hf	-907.15	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	83.24	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.403		Crippen Method
mcvol	308.920	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	866.56	K	Joback Method
tc	1067.96	K	Joback Method
tf	496.78	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.22	J/mol×K	866.56	Joback Method
cpg	1014.84	J/mol×K	900.13	Joback Method
cpg	1031.14	J/mol×K	933.69	Joback Method
cpg	1046.13	J/mol×K	967.26	Joback Method
cpg	1059.85	J/mol×K	1000.82	Joback Method
cpg	1072.33	J/mol×K	1034.39	Joback Method
cpg	1083.59	J/mol×K	1067.96	Joback Method
dvisc	0.0007505	Pa×s	496.78	Joback Method

dvisc	0.0003665	Pa×s	558.41	Joback Method
dvisc	0.0002064	Pa×s	620.04	Joback Method
dvisc	0.0001290	Pa×s	681.67	Joback Method
dvisc	0.0000871	Pa×s	743.30	Joback Method
dvisc	0.0000625	Pa×s	804.93	Joback Method
dvisc	0.0000470	Pa×s	866.56	Joback Method

Sources

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=U393465&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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