Glutaric acid, 8-chlorooctyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C20H28Cl2O5/c1-25-18-15-16(22)11-12-17(18)27-20(24)10-8-9-19(23)26-14-7

InchiKey: ZWKWDSSOOMCJLM-UHFFFAOYSA-N

Formula: C20H28Cl2O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 419.34

Physical Properties

Property code	Value	Unit	Source
gf	-386.03	kJ/mol	Joback Method
hf	-895.84	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	93.21	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.547		Crippen Method
mcvol	314.130	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	943.50	K	Joback Method
tc	1158.06	K	Joback Method
tf	593.01	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.63	J/mol×K	943.50	Joback Method
cpg	1008.64	J/mol×K	1122.30	Joback Method
cpg	1000.85	J/mol×K	1086.54	Joback Method
cpg	991.77	J/mol×K	1050.78	Joback Method
cpg	981.38	J/mol×K	1015.02	Joback Method
cpg	969.67	J/mol×K	979.26	Joback Method
cpg	1015.13	J/mol×K	1158.06	Joback Method
dvisc	0.0000304	Pa×s	943.50	Joback Method

dvisc	0.0000383	Pa×s	885.09	Joback Method
dvisc	0.0000500	Pa×s	826.67	Joback Method
dvisc	0.0000678	Pa×s	768.25	Joback Method
dvisc	0.0000969	Pa×s	709.84	Joback Method
dvisc	0.0001475	Pa×s	651.42	Joback Method
dvisc	0.0002439	Pa×s	593.01	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=U393914&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