Glutaric acid, 8-chlorooctyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C19H25Cl3O4/c20-13-5-3-1-2-4-6-14-25-17(23)11-8-12-18(24)26-16-10-7-9-15

InchiKey: YMDOBJNWMYJWQB-UHFFFAOYSA-N

Formula: C19H25Cl3O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCCCCCCCCCCl

Mol. weight [g/mol]: 423.76

Physical Properties

Property code	Value	Unit	Source
gf	-301.38	kJ/mol	Joback Method
hf	-758.72	kJ/mol	Joback Method
hfus	56.39	kJ/mol	Joback Method
hvap	92.95	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.192		Crippen Method
mcvol	306.410	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	3084.00		NIST Webbook
rinpol	3084.00		NIST Webbook
tb	935.63	K	Joback Method
tc	1151.62	K	Joback Method
tf	589.43	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.57	J/mol×K	935.63	Joback Method
cpg	905.90	J/mol×K	971.63	Joback Method
cpg	917.07	J/mol×K	1007.63	Joback Method
cpg	927.11	J/mol×K	1043.62	Joback Method
cpg	936.05	J/mol×K	1079.62	Joback Method
cpg	943.90	J/mol×K	1115.62	Joback Method
cpg	950.69	J/mol×K	1151.62	Joback Method
dvisc	0.0003161	Pa×s	589.43	Joback Method

dvisc	0.0001924	Pa×s	647.13	Joback Method
dvisc	0.0001270	Pa×s	704.83	Joback Method
dvisc	0.0000893	Pa×s	762.53	Joback Method
dvisc	0.0000660	Pa×s	820.23	Joback Method
dvisc	0.0000507	Pa×s	877.93	Joback Method
dvisc	0.0000403	Pa×s	935.63	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=U391993&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