Glutaric acid, 8-chlorooctyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C19H25Cl2FO4/c20-13-5-3-1-2-4-6-14-25-17(23)11-8-12-18(24)26-19-15(21)9

InchiKey: CGATXVMRULGOQR-UHFFFAOYSA-N

Formula: C19H25Cl2FO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCCCCCCCCCCl

Mol. weight [g/mol]: 407.30

Physical Properties

Property code	Value	Unit	Source
gf	-484.26	kJ/mol	Joback Method
hf	-939.09	kJ/mol	Joback Method
hfus	55.28	kJ/mol	Joback Method
hvap	87.75	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.677		Crippen Method
mcvol	295.940	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	2838.00		NIST Webbook
rinpol	2838.00		NIST Webbook
tb	897.47	K	Joback Method
tc	1104.54	K	Joback Method
tf	560.10	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.66	J/mol×K	897.47	Joback Method
cpg	890.84	J/mol×K	931.98	Joback Method
cpg	902.91	J/mol×K	966.49	Joback Method
cpg	913.91	J/mol×K	1001.00	Joback Method
cpg	923.84	J/mol×K	1035.52	Joback Method
cpg	932.74	J/mol×K	1070.03	Joback Method
cpg	940.62	J/mol×K	1104.54	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=U391590&Units=SI

Legend

cpg:	Ideal gas heat capacity
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