Glutaric acid, 8-chlorooctyl 3-fluorophenyl ester

Inchi: InChI=1S/C19H26ClFO4/c20-13-5-3-1-2-4-6-14-24-18(22)11-8-12-19(23)25-17-10-7-9-1

InchiKey: XINNFEKEKKTZQS-UHFFFAOYSA-N

Formula: C19H26ClFO4

SMILES: O=C(CCCC(=O)Oc1cccc(F)c1)OCCCCCCCCCCl

Mol. weight [g/mol]: 372.86

Physical Properties

Property code	Value	Unit	Source
gf	-462.70	kJ/mol	Joback Method
hf	-911.88	kJ/mol	Joback Method
hfus	51.47	kJ/mol	Joback Method
hvap	82.71	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.024		Crippen Method
mcvol	283.700	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2678.00		NIST Webbook
rinpol	2678.00		NIST Webbook
tb	855.06	K	Joback Method
tc	1055.52	K	Joback Method
tf	517.66	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.63	J/mol×K	855.06	Joback Method
cpg	868.00	J/mol×K	888.47	Joback Method
cpg	881.31	J/mol×K	921.88	Joback Method
cpg	893.56	J/mol×K	955.29	Joback Method
cpg	904.80	J/mol×K	988.70	Joback Method
cpg	915.03	J/mol×K	1022.11	Joback Method
cpg	924.29	J/mol×K	1055.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392098&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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