Glutaric acid, 3,3,4,4-tetrafluoropropyl 10-chlorodecyl ester

Inchi: InChI=1S/C18H29ClF4O4/c19-12-7-5-3-1-2-4-6-8-13-26-15(24)10-9-11-16(25)27-14-18(
InchiKey: NSAYNXXWHCAZKD-UHFFFAOYSA-N
Formula: C18H29ClF4O4
SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCCCCCCCCCCCCl
Mol. weight [g/mol]: 420.87

Physical Properties

Property code	Value	Unit	Source
gf	-1157.93	kJ/mol	Joback Method
hf	-1718.66	kJ/mol	Joback Method
hfus	53.53	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.503		Crippen Method
mcvol	298.680	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	794.66	K	Joback Method
tc	973.98	K	Joback Method
tf	456.64	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.91	J/mol×K	794.66	Joback Method
cpg	928.38	J/mol×K	824.55	Joback Method
cpg	942.94	J/mol×K	854.43	Joback Method
cpg	956.60	J/mol×K	884.32	Joback Method
cpg	969.39	J/mol×K	914.21	Joback Method
cpg	981.35	J/mol×K	944.09	Joback Method
cpg	992.49	J/mol×K	973.98	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=U392451&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