Glutaric acid, 8-chlorooctyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C17H25ClF6O4/c18-10-5-3-1-2-4-6-11-27-13(25)8-7-9-14(26)28-12-16(20,21)1

InchiKey: KHXYEXRJSIGLSM-UHFFFAOYSA-N

Formula: C17H25ClF6O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)C(F)(F)F)OCCCCCCCCCl

Mol. weight [g/mol]: 442.82

Physical Properties

Property code	Value	Unit	Source
gf	-1553.13	kJ/mol	Joback Method
hf	-2098.99	kJ/mol	Joback Method
hfus	49.69	kJ/mol	Joback Method
hvap	68.25	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.358		Crippen Method
mcvol	288.130	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
tb	767.09	K	Joback Method
tc	940.90	K	Joback Method
tf	448.97	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.89	J/mol×K	767.09	Joback Method
cpg	886.31	J/mol×K	796.06	Joback Method
cpg	899.87	J/mol×K	825.03	Joback Method
cpg	912.61	J/mol×K	854.00	Joback Method
cpg	924.56	J/mol×K	882.97	Joback Method
cpg	935.76	J/mol×K	911.93	Joback Method
cpg	946.25	J/mol×K	940.90	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=U393696&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