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

Inchi: InChI=1S/C16H24ClF5O4/c17-10-5-3-1-2-4-6-11-25-13(23)8-7-9-14(24)26-12-15(18,19)1

InchiKey: ANKTVYCEBQSQOI-UHFFFAOYSA-N

Formula: C16H24ClF5O4

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

Mol. weight [g/mol]: 410.80

Physical Properties

Property code	Value	Unit	Source
gf	-1364.30	kJ/mol	Joback Method
hf	-1876.96	kJ/mol	Joback Method
hfus	47.54	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.020		Crippen Method
mcvol	272.270	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	745.38	K	Joback Method
tc	917.55	K	Joback Method
tf	452.11	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.07	J/mol×K	745.38	Joback Method
cpg	821.17	J/mol×K	774.08	Joback Method
cpg	834.45	J/mol×K	802.77	Joback Method
cpg	846.95	J/mol×K	831.47	Joback Method
cpg	858.71	J/mol×K	860.16	Joback Method
cpg	869.75	J/mol×K	888.86	Joback Method
cpg	880.11	J/mol×K	917.55	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=U393679&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