Glutaric acid, cyclohexylmethyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C16H22F6O4/c17-14(16(20,21)22)15(18,19)10-26-13(24)8-4-7-12(23)25-9-11-

InchiKey: MHMOOVIVLUBWLI-UHFFFAOYSA-N

Formula: C16H22F6O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)C(F)(F)F)OCC1CCCCC1

Mol. weight [g/mol]: 392.33

Physical Properties

Property code	Value	Unit	Source
gf	-1525.17	kJ/mol	Joback Method
hf	-2008.29	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.359		Crippen Method
mcvol	250.940	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	1809.00		NIST Webbook
rinpol	1809.00		NIST Webbook
tb	726.33	K	Joback Method
tc	905.14	K	Joback Method
tf	415.16	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.64	J/mol×K	726.33	Joback Method
cpg	795.54	J/mol×K	756.13	Joback Method
cpg	810.42	J/mol×K	785.93	Joback Method
cpg	824.32	J/mol×K	815.73	Joback Method
cpg	837.28	J/mol×K	845.53	Joback Method
cpg	849.34	J/mol×K	875.33	Joback Method
cpg	860.53	J/mol×K	905.14	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=U393691&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