Glutaric acid, 2,2,3,3,4,4,4-heptafluorobutyl propyl ester

Inchi: InChI=1S/C12H15F7O4/c1-2-6-22-8(20)4-3-5-9(21)23-7-10(13,14)11(15,16)12(17,18)19/

InchiKey: AZSFHNCOPRRXAT-UHFFFAOYSA-N

Formula: C12H15F7O4

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

Mol. weight [g/mol]: 356.23

Physical Properties

Property code	Value	Unit	Source
gf	-1772.83	kJ/mol	Joback Method
hf	-2179.63	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.486		Crippen Method
mcvol	207.210	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	1443.00		NIST Webbook
tb	611.74	K	Joback Method
tc	769.46	K	Joback Method
tf	380.71	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.56	J/mol×K	611.74	Joback Method
cpg	594.05	J/mol×K	638.03	Joback Method
cpg	605.84	J/mol×K	664.31	Joback Method
cpg	616.96	J/mol×K	690.60	Joback Method
cpg	627.45	J/mol×K	716.89	Joback Method
cpg	637.32	J/mol×K	743.18	Joback Method
cpg	646.60	J/mol×K	769.46	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=U377546&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