Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C13H11F13O4/c14-8(15)11(20,21)12(22,23)9(16,17)4-29-6(27)2-1-3-7(28)30-5

InchiKey: YBCNCCRUDNJINL-UHFFFAOYSA-N

Formula: C13H11F13O4

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

Mol. weight [g/mol]: 478.20

Physical Properties

Property code	Value	Unit	Source
gf	-2930.03	kJ/mol	Joback Method
hf	-3399.71	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	45.35	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.612		Crippen Method
mcvol	231.920	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	623.34	K	Joback Method
tc	769.82	K	Joback Method
tf	385.36	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.62	J/mol×K	623.34	Joback Method
cpg	699.37	J/mol×K	647.75	Joback Method
cpg	710.37	J/mol×K	672.17	Joback Method
cpg	720.66	J/mol×K	696.58	Joback Method
cpg	730.27	J/mol×K	721.00	Joback Method
cpg	739.26	J/mol×K	745.41	Joback Method
cpg	747.64	J/mol×K	769.82	Joback Method

Sources

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=U393665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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