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

Inchi: InChI=1S/C14H18F8O4/c1-2-3-7-25-9(23)5-4-6-10(24)26-8-12(17,18)14(21,22)13(19,20)

InchiKey: LYPAMHBKYJXVLJ-UHFFFAOYSA-N

Formula: C14H18F8O4

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

Mol. weight [g/mol]: 402.28

Physical Properties

Property code	Value	Unit	Source
gf	-1953.24	kJ/mol	Joback Method
hf	-2422.30	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.214		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	656.33	K	Joback Method
tc	813.73	K	Joback Method
tf	388.84	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.10	J/mol×K	656.33	Joback Method
cpg	707.36	J/mol×K	682.56	Joback Method
cpg	719.88	J/mol×K	708.80	Joback Method
cpg	731.69	J/mol×K	735.03	Joback Method
cpg	742.81	J/mol×K	761.27	Joback Method
cpg	753.29	J/mol×K	787.50	Joback Method
cpg	763.16	J/mol×K	813.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359678&Units=SI
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

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