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

Inchi: InChI=1S/C13H17F7O4/c1-2-3-7-23-9(21)5-4-6-10(22)24-8-11(14,15)12(16,17)13(18,19)

InchiKey: QSOOQBSMLHTGJM-UHFFFAOYSA-N

Formula: C13H17F7O4

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

Mol. weight [g/mol]: 370.26

Physical Properties

Property code	Value	Unit	Source
gf	-1764.41	kJ/mol	Joback Method
hf	-2200.27	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.876		Crippen Method
mcvol	221.300	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
tb	634.62	K	Joback Method
tc	793.03	K	Joback Method
tf	391.98	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.98	J/mol×K	634.62	Joback Method
cpg	645.95	J/mol×K	661.02	Joback Method
cpg	658.21	J/mol×K	687.42	Joback Method
cpg	669.77	J/mol×K	713.83	Joback Method
cpg	680.67	J/mol×K	740.23	Joback Method
cpg	690.94	J/mol×K	766.63	Joback Method
cpg	700.61	J/mol×K	793.03	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=U377548&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

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