Glutaric acid, hex-4-yn-3-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H18F6O4/c1-3-6-10(4-2)25-12(23)8-5-7-11(22)24-9-14(17,18)13(16)15(19

InchiKey: CZDOPFKQQCJCDG-UHFFFAOYSA-N

Formula: C15H18F6O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 376.29

Physical Properties

Property code	Value	Unit	Source
gf	-1357.68	kJ/mol	Joback Method
hf	-1774.95	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.581		Crippen Method
mcvol	239.110	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
tb	692.46	K	Joback Method
tc	866.65	K	Joback Method
tf	487.61	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.01	J/mol×K	692.46	Joback Method
cpg	699.54	J/mol×K	721.49	Joback Method
cpg	712.29	J/mol×K	750.52	Joback Method
cpg	724.28	J/mol×K	779.55	Joback Method
cpg	735.53	J/mol×K	808.58	Joback Method
cpg	746.09	J/mol×K	837.62	Joback Method
cpg	755.97	J/mol×K	866.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393687&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume