Glutaric acid, hex-4-yn-3-yl pentafluorobenzyl ester

Inchi: InChI=1S/C18H17F5O4/c1-3-6-10(4-2)27-13(25)8-5-7-12(24)26-9-11-14(19)16(21)18(23

InchiKey: HFXPEDGNKPYJCL-UHFFFAOYSA-N

Formula: C18H17F5O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 392.32

Physical Properties

Property code	Value	Unit	Source
gf	-1076.59	kJ/mol	Joback Method
hf	-1438.80	kJ/mol	Joback Method
hfus	55.05	kJ/mol	Joback Method
hvap	77.24	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	3.941		Crippen Method
mcvol	255.850	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tb	820.31	K	Joback Method
tc	1014.01	K	Joback Method
tf	620.01	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.41	J/mol×K	820.31	Joback Method
cpg	757.99	J/mol×K	852.59	Joback Method
cpg	769.69	J/mol×K	884.88	Joback Method
cpg	780.48	J/mol×K	917.16	Joback Method
cpg	790.37	J/mol×K	949.45	Joback Method
cpg	799.36	J/mol×K	981.73	Joback Method
cpg	807.44	J/mol×K	1014.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391932&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume