Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl non-5-yn-3-yl ester

Inchi: InChI=1S/C19H24F8O4/c1-3-5-6-7-9-13(4-2)31-15(29)11-8-10-14(28)30-12-17(22,23)19

InchiKey: SHYKAIPCNOSAMT-UHFFFAOYSA-N

Formula: C19H24F8O4

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

Mol. weight [g/mol]: 468.38

Physical Properties

Property code	Value	Unit	Source
gf	-1710.78	kJ/mol	Joback Method
hf	-2258.48	kJ/mol	Joback Method
hfus	49.01	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.386		Crippen Method
mcvol	299.010	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	779.29	K	Joback Method
tc	956.75	K	Joback Method
tf	536.29	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.25	J/mol×K	779.29	Joback Method
cpg	940.86	J/mol×K	808.87	Joback Method
cpg	954.56	J/mol×K	838.44	Joback Method
cpg	967.40	J/mol×K	868.02	Joback Method
cpg	979.42	J/mol×K	897.59	Joback Method
cpg	990.69	J/mol×K	927.17	Joback Method
cpg	1001.25	J/mol×K	956.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393950&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