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

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

InchiKey: QOXLPCQGVJIHPF-UHFFFAOYSA-N

Formula: C19H24F8O4

SMILES: CCC#CC(CC(C)C)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	-1713.22	kJ/mol	Joback Method
hf	-2263.76	kJ/mol	Joback Method
hfus	45.49	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.242		Crippen Method
mcvol	299.010	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	1844.00		NIST Webbook
rinpol	1844.00		NIST Webbook
tb	778.85	K	Joback Method
tc	957.09	K	Joback Method
tf	521.29	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.78	J/mol×K	778.85	Joback Method
cpg	941.46	J/mol×K	808.56	Joback Method
cpg	955.22	J/mol×K	838.26	Joback Method
cpg	968.10	J/mol×K	867.97	Joback Method
cpg	980.15	J/mol×K	897.68	Joback Method
cpg	991.43	J/mol×K	927.38	Joback Method
cpg	1001.98	J/mol×K	957.09	Joback Method

Sources

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=U394016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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