Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C21H26F8O4/c1-5-7-14(4)15(11-10-13(2)3)33-17(31)9-6-8-16(30)32-12-19(24

InchiKey: ZIVDKJOSFYMTSI-UHFFFAOYSA-N

Formula: C21H26F8O4

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

Mol. weight [g/mol]: 494.42

Physical Properties

Property code	Value	Unit	Source
gf	-1617.09	kJ/mol	Joback Method
hf	-2189.40	kJ/mol	Joback Method
hfus	48.08	kJ/mol	Joback Method
hvap	70.63	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.798		Crippen Method
mcvol	322.890	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	821.17	K	Joback Method
tc	1006.61	K	Joback Method
tf	528.11	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.88	J/mol×K	821.17	Joback Method
cpg	1030.89	J/mol×K	852.08	Joback Method
cpg	1044.93	J/mol×K	882.98	Joback Method
cpg	1058.07	J/mol×K	913.89	Joback Method
cpg	1070.37	J/mol×K	944.80	Joback Method
cpg	1081.90	J/mol×K	975.71	Joback Method
cpg	1092.71	J/mol×K	1006.61	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=U393961&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