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

Inchi: InChI=1S/C19H26F4O4/c1-5-7-14(4)15(11-10-13(2)3)27-17(25)9-6-8-16(24)26-12-19(22
InchiKey: HRSPCHSRZDDBNL-UHFFFAOYSA-N
Formula: C19H26F4O4
SMILES: C=C(C)C#CC(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)C(C)CCC
Mol. weight [g/mol]: 394.40

Physical Properties

Property code	Value	Unit	Source
gf	-860.37	kJ/mol	Joback Method
hf	-1346.18	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.528		Crippen Method
mcvol	287.630	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	784.79	K	Joback Method
tc	970.40	K	Joback Method
tf	498.37	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.88	J/mol×K	784.79	Joback Method
cpg	882.36	J/mol×K	815.73	Joback Method
cpg	896.89	J/mol×K	846.66	Joback Method
cpg	910.51	J/mol×K	877.60	Joback Method
cpg	923.25	J/mol×K	908.53	Joback Method
cpg	935.14	J/mol×K	939.47	Joback Method
cpg	946.21	J/mol×K	970.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393960&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