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

Inchi: InChI=1S/C19H27F3O4/c1-6-8-14(4)16(12-11-13(2)3)26-18(24)10-7-9-17(23)25-15(5)19

InchiKey: OJKCVMUEEITITK-UHFFFAOYSA-N

Formula: C19H27F3O4

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

Mol. weight [g/mol]: 376.41

Physical Properties

Property code	Value	Unit	Source
gf	-665.56	kJ/mol	Joback Method
hf	-1150.07	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.578		Crippen Method
mcvol	285.860	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
tb	785.52	K	Joback Method
tc	975.06	K	Joback Method
tf	497.78	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.31	J/mol×K	785.52	Joback Method
cpg	875.21	J/mol×K	817.11	Joback Method
cpg	890.12	J/mol×K	848.70	Joback Method
cpg	904.09	J/mol×K	880.29	Joback Method
cpg	917.14	J/mol×K	911.88	Joback Method
cpg	929.31	J/mol×K	943.47	Joback Method
cpg	940.63	J/mol×K	975.06	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=U393959&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