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

Inchi: InChI=1S/C18H19F3O2/c1-5-6-12(4)15(10-7-11(2)3)23-18(22)13-8-9-14(19)17(21)16(13

InchiKey: CBPQGJKFGCIMQC-UHFFFAOYSA-N

Formula: C18H19F3O2

SMILES: C=C(C)C#CC(OC(=O)c1ccc(F)c(F)c1F)C(C)CCC

Mol. weight [g/mol]: 324.34

Physical Properties

Property code	Value	Unit	Source
gf	-356.94	kJ/mol	Joback Method
hf	-668.48	kJ/mol	Joback Method
hfus	40.76	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.645		Crippen Method
mcvol	240.570	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	1815.30		NIST Webbook
rinpol	1815.30		NIST Webbook
tb	731.64	K	Joback Method
tc	933.12	K	Joback Method
tf	490.91	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.01	J/mol×K	731.64	Joback Method
cpg	678.21	J/mol×K	765.22	Joback Method
cpg	692.49	J/mol×K	798.80	Joback Method
cpg	705.88	J/mol×K	832.38	Joback Method
cpg	718.41	J/mol×K	865.96	Joback Method
cpg	730.09	J/mol×K	899.54	Joback Method
cpg	740.95	J/mol×K	933.12	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=U292558&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