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

Inchi: InChI=1S/C19H21F3O2/c1-5-8-14(4)17(12-11-13(2)3)24-18(23)15-9-6-7-10-16(15)19(20

InchiKey: RSQXEBKVKNSXNK-UHFFFAOYSA-N

Formula: C19H21F3O2

SMILES: C=C(C)C#CC(OC(=O)c1ccccc1C(F)(F)F)C(C)CCC

Mol. weight [g/mol]: 338.36

Physical Properties

Property code	Value	Unit	Source
gf	-326.42	kJ/mol	Joback Method
hf	-674.93	kJ/mol	Joback Method
hfus	36.72	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.247		Crippen Method
mcvol	254.660	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	1832.00		NIST Webbook
tb	741.33	K	Joback Method
tc	947.92	K	Joback Method
tf	479.56	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.85	J/mol×K	741.33	Joback Method
cpg	737.97	J/mol×K	775.76	Joback Method
cpg	753.02	J/mol×K	810.19	Joback Method
cpg	767.05	J/mol×K	844.62	Joback Method
cpg	780.13	J/mol×K	879.06	Joback Method
cpg	792.32	J/mol×K	913.49	Joback Method
cpg	803.66	J/mol×K	947.92	Joback Method

Sources

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=U299407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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