2,3,4-Trifluorobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H17F3O2/c1-4-5-6-11(9-10(2)3)21-16(20)12-7-8-13(17)15(19)14(12)18/h7
InchiKey: YMDLHXAODPRPKL-UHFFFAOYSA-N
Formula: C16H17F3O2
SMILES: CCC#CC(CC(C)C)OC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 298.30

Physical Properties

Property code	Value	Unit	Source
gf	-453.07	kJ/mol	Joback Method
hf	-742.84	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	63.55	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.089		Crippen Method
mcvol	216.690	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	1698.40		NIST Webbook
rinpol	1698.40		NIST Webbook
tb	689.32	K	Joback Method
tc	889.18	K	Joback Method
tf	484.09	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.49	J/mol×K	689.32	Joback Method
cpg	594.25	J/mol×K	722.63	Joback Method
cpg	608.16	J/mol×K	755.94	Joback Method
cpg	621.26	J/mol×K	789.25	Joback Method
cpg	633.54	J/mol×K	822.56	Joback Method
cpg	645.02	J/mol×K	855.87	Joback Method
cpg	655.72	J/mol×K	889.18	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=U292556&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

Latest version available from:
https://www.chemeo.com/cid/120-671-3/2-3-4-Trifluorobenzoic-acid-2-methyloct-5-yn-4-yl-ester.pdf
Generated by Cheméo on 2024-10-12 09:37:25.824303065 +0000 UTC m=+3306708.461272314.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.