

4-(Trifluoromethyl)benzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C17H19F3O2/c1-4-5-6-15(11-12(2)3)22-16(21)13-7-9-14(10-8-13)17(18,19)20
InchiKey:	DVPQLGWTAQYDJJ-UHFFFAOYSA-N
Formula:	C17H19F3O2
SMILES:	CCC#CC(CC(C)C)OC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	312.33

Physical Properties

Property code	Value	Unit	Source
gf	-422.55	kJ/mol	Joback Method
hf	-749.29	kJ/mol	Joback Method
hfus	34.13	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.690		Crippen Method
mcvol	230.780	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinsol	1669.00		NIST Webbook
tb	699.01	K	Joback Method
tc	904.33	K	Joback Method
tf	472.74	K	Joback Method
vc	0.896	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.00	J/mol×K	699.01	Joback Method
cpg	652.91	J/mol×K	733.23	Joback Method
cpg	667.77	J/mol×K	767.45	Joback Method
cpg	681.65	J/mol×K	801.67	Joback Method
cpg	694.58	J/mol×K	835.89	Joback Method
cpg	706.62	J/mol×K	870.11	Joback Method
cpg	717.80	J/mol×K	904.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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

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