Trichloroacetic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C11H15Cl3O2/c1-4-5-6-9(7-8(2)3)16-10(15)11(12,13)14/h8-9H,4,7H2,1-3H3
InchiKey: BFHVFJFRDWWLLF-UHFFFAOYSA-N
Formula: C11H15Cl3O2
SMILES: CCC#CC(CC(C)C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 285.60

Physical Properties

Property code	Value	Unit	Source
gf	-27.21	kJ/mol	Joback Method
hf	-309.40	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.728		Crippen Method
mcvol	201.410	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1500.00		NIST Webbook
tb	644.55	K	Joback Method
tc	868.09	K	Joback Method
tf	454.17	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.22	J/mol×K	644.55	Joback Method
cpg	479.47	J/mol×K	681.81	Joback Method
cpg	491.83	J/mol×K	719.06	Joback Method
cpg	503.34	J/mol×K	756.32	Joback Method
cpg	514.04	J/mol×K	793.57	Joback Method
cpg	523.98	J/mol×K	830.83	Joback Method
cpg	533.19	J/mol×K	868.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U299258&Units=SI

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

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