1,6-Heptadien-4-ol, trifluoroacetate

Inchi: InChI=1S/C9H11F3O2/c1-3-5-7(6-4-2)14-8(13)9(10,11)12/h3-4,7H,1-2,5-6H2
InchiKey: VOIOLVJUKBWWLY-UHFFFAOYSA-N
Formula: C9H11F3O2
SMILES: C=CCC(CC=C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 208.18

Physical Properties

Property code	Value	Unit	Source
gf	-617.37	kJ/mol	Joback Method
hf	-825.39	kJ/mol	Joback Method
hfus	17.60	kJ/mol	Joback Method
hvap	39.31	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.613		Crippen Method
mcvol	141.820	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	846.30		NIST Webbook
rinpol	846.30		NIST Webbook
tb	469.11	K	Joback Method
tc	637.79	K	Joback Method
tf	249.02	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.04	J/mol×K	469.11	Joback Method
cpg	327.78	J/mol×K	497.22	Joback Method
cpg	338.93	J/mol×K	525.34	Joback Method
cpg	349.51	J/mol×K	553.45	Joback Method
cpg	359.53	J/mol×K	581.56	Joback Method
cpg	369.03	J/mol×K	609.68	Joback Method
cpg	378.01	J/mol×K	637.79	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=U352759&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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