Cycloheptanol, trifluoroacetate

Inchi: InChI=1S/C9H13F3O2/c10-9(11,12)8(13)14-7-5-3-1-2-4-6-7/h7H,1-6H2
InchiKey: VKBULDZQMPQVFH-UHFFFAOYSA-N
Formula: C9H13F3O2
SMILES: O=C(OC1CCCCCC1)C(F)(F)F
Mol. weight [g/mol]: 210.19

Physical Properties

Property code	Value	Unit	Source
gf	-778.26	kJ/mol	Joback Method
hf	-1022.81	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	41.64	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.815		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1019.00		NIST Webbook
tb	500.01	K	Joback Method
tc	697.11	K	Joback Method
tf	271.40	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.93	J/mol×K	500.01	Joback Method
cpg	352.70	J/mol×K	532.86	Joback Method
cpg	368.54	J/mol×K	565.71	Joback Method
cpg	383.47	J/mol×K	598.56	Joback Method
cpg	397.52	J/mol×K	631.41	Joback Method
cpg	410.69	J/mol×K	664.26	Joback Method
cpg	423.03	J/mol×K	697.11	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=U376258&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