Acetic acid, trifluoro-, cyclohexyl ester

Other names: Trifluoroacetic acid, cyclohexyl ester
Inchi: InChI=1S/C8H11F3O2/c9-8(10,11)7(12)13-6-4-2-1-3-5-6/h6H,1-5H2
InchiKey: MJNDVDVTLSBDLB-UHFFFAOYSA-N
Formula: C8H11F3O2
SMILES: O=C(OC1CCCCC1)C(F)(F)F
Mol. weight [g/mol]: 196.17
CAS: 1549-45-7

Physical Properties

Property code	Value	Unit	Source
gf	-774.58	kJ/mol	Joback Method
hf	-996.01	kJ/mol	Joback Method
hfus	12.92	kJ/mol	Joback Method
hvap	39.24	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.425		Crippen Method
mcvol	125.470	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
tb	472.86	K	Joback Method
tc	665.20	K	Joback Method
tf	263.65	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.97	J/mol×K	633.14	Joback Method
cpg	290.69	J/mol×K	472.86	Joback Method
cpg	305.76	J/mol×K	504.92	Joback Method
cpg	320.00	J/mol×K	536.97	Joback Method
cpg	333.43	J/mol×K	569.03	Joback Method
cpg	346.08	J/mol×K	601.09	Joback Method
cpg	369.12	J/mol×K	665.20	Joback Method
hvapt	43.00	kJ/mol	382.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57944e+01
Coeff. B	-4.38827e+03
Coeff. C	-2.83500e+01
Temperature range (K), min.	311.34
Temperature range (K), max.	446.96

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=C1549457&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume