O-Trifluoroacetyl-menthol

Other names: Trifluoroacetyl-menthol
Menthol, trifluoroacetate
Inchi: InChI=1S/C12H19F3O2/c1-7(2)9-5-4-8(3)6-10(9)17-11(16)12(13,14)15/h7-10H,4-6H2,1-
InchiKey: ATXCXBAHNZQECW-UHFFFAOYSA-N
Formula: C12H19F3O2
SMILES: CC1CCC(C(C)C)C(OC(=O)C(F)(F)F)C1
Mol. weight [g/mol]: 252.27
CAS: 28587-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-758.76	kJ/mol	Joback Method
hf	-1124.53	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	47.14	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.553		Crippen Method
mcvol	181.830	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
tb	554.60	K	Joback Method
tc	741.49	K	Joback Method
tf	285.25	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.28	J/mol×K	554.60	Joback Method
cpg	502.11	J/mol×K	585.75	Joback Method
cpg	519.96	J/mol×K	616.90	Joback Method
cpg	536.85	J/mol×K	648.05	Joback Method
cpg	552.81	J/mol×K	679.19	Joback Method

cpg	567.86	J/mol×K	710.34	Joback Method
cpg	582.01	J/mol×K	741.49	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=C28587500&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