3-(Trifluoroacetyl)-D-camphor

Other names: Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-3-(trifluoroacetyl)-, (1R)-
(1R)-1,7,7-trimethyl-3-(trifluoroacetyl)bicyclo[2.2.1]heptan-2-one
Inchi: InChI=1S/C12H15F3O2/c1-10(2)6-4-5-11(10,3)8(16)7(6)9(17)12(13,14)15/h6-7H,4-5H2,
InchiKey: ISLOIHOAZDSEAJ-UHFFFAOYSA-N
Formula: C12H15F3O2
SMILES: CC12CCC(C(C(=O)C(F)(F)F)C1=O)C2(C)C
Mol. weight [g/mol]: 248.24
CAS: 51800-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-699.94	kJ/mol	Joback Method
hf	-1009.13	kJ/mol	Joback Method
hfus	13.49	kJ/mol	Joback Method
hvap	46.63	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.759		Crippen Method
mcvol	166.670	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
tb	599.12	K	Joback Method
tc	811.99	K	Joback Method
tf	419.02	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.86	J/mol×K	599.12	Joback Method
cpg	488.34	J/mol×K	634.60	Joback Method
cpg	503.82	J/mol×K	670.08	Joback Method
cpg	518.50	J/mol×K	705.55	Joback Method
cpg	532.61	J/mol×K	741.03	Joback Method
cpg	546.37	J/mol×K	776.51	Joback Method
cpg	559.97	J/mol×K	811.99	Joback Method

Sources

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=C51800987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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