3-Heptafluorobutyryl-«delta»-camphor

Other names:	3-(Heptafluorobutyryl)-D-camphor
	Bicyclo[2.2.1]heptan-2-one, 3-(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)-1,7,7-trimethyl-, (1R)-
	3-Heptafluorobutyryl-(+)-camphor
	(1R)-3-(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one
Inchi:	InChI=1S/C14H15F7O2/c1-10(2)6-4-5-11(10,3)8(22)7(6)9(23)12(15,16)13(17,18)14(19,2
InchiKey:	PEWOESYEGLBLNR-UHFFFAOYSA-N
Formula:	C14H15F7O2
SMILES:	CC12CCC(C(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C1=O)C2(C)C
Mol. weight [g/mol]:	348.26
CAS:	51800-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-1456.66	kJ/mol	Joback Method
hf	-1852.35	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.030		Crippen Method
mcvol	201.930	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
tb	635.50	K	Joback Method
tc	828.57	K	Joback Method
tf	448.76	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.54	J/mol×K	635.50	Joback Method
cpg	628.39	J/mol×K	667.68	Joback Method
cpg	643.29	J/mol×K	699.86	Joback Method
cpg	657.45	J/mol×K	732.03	Joback Method
cpg	671.05	J/mol×K	764.21	Joback Method

cpg	684.30	J/mol×K	796.39	Joback Method
cpg	697.41	J/mol×K	828.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.20	K	0.03	NIST Webbook

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=C51800998&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume