

3-HEPTAFLUOROBUTYRYL-(+)-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(19,20)
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

Physical Properties

Property code	Value	Unit	Source
hfus	16.16	kJ/mol	Joback Method
logp	4.030		Crippen Method
mcvol	201.930	ml/mol	McGowan 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51800998&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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