

Endo-2,2,3,3-tetrafluoro-5-methylbicyclo[2.1.0]pentane

Inchi:	InChI=1S/C6H6F4/c1-2-3-4(2)6(9,10)5(3,7)8/h2-4H,1H3/t2-,3-,4+
InchiKey:	YBDXROWBSCGEOB-JANPFBAGSA-N
Formula:	C6H6F4
SMILES:	CC1C2C1C(F)(F)C2(F)F
Mol. weight [g/mol]:	154.11
CAS:	87102-52-1

Physical Properties

Property code	Value	Unit	Source
gf	-680.11	kJ/mol	Joback Method
hf	-830.39	kJ/mol	Joback Method
hfus	12.60	kJ/mol	Joback Method
hvap	22.11	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.153		Crippen Method
mcvol	80.760	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	329.44	K	Joback Method
tc	489.39	K	Joback Method
tf	234.22	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.63	J/mol×K	329.44	Joback Method
cpg	170.61	J/mol×K	356.10	Joback Method
cpg	183.34	J/mol×K	382.76	Joback Method
cpg	194.92	J/mol×K	409.41	Joback Method
cpg	205.45	J/mol×K	436.07	Joback Method
cpg	215.01	J/mol×K	462.73	Joback Method
cpg	223.70	J/mol×K	489.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C87102521&Units=SI

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

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