

«alpha»-(Trifluoromethoxy)-«alpha»,«alpha»-difluoroacetate

Inchi: InChI=1S/C4H3F5O3/c1-2(10)11-4(8,9)12-3(5,6)7/h1H3

InchiKey: LMIXDPWHHJAXJJ-UHFFFAOYSA-N

Formula: C4H3F5O3

SMILES: CC(=O)OC(F)(F)OC(F)(F)F

Mol. weight [g/mol]: 194.06

CAS: 2195-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-1324.49	kJ/mol	Joback Method
hf	-1500.96	kJ/mol	Joback Method
hfus	10.66	kJ/mol	Joback Method
hvap	29.39	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.636		Crippen Method
mvol	89.380	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	379.52	K	Joback Method
tc	535.07	K	Joback Method
tf	237.02	K	Joback Method
vc	0.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.42	J/molxK	379.52	Joback Method
cpg	201.78	J/molxK	405.45	Joback Method
cpg	208.79	J/molxK	431.37	Joback Method
cpg	215.44	J/molxK	457.30	Joback Method
cpg	221.75	J/molxK	483.22	Joback Method
cpg	227.72	J/molxK	509.15	Joback Method
cpg	233.37	J/molxK	535.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2195848&Units=SI
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

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
mccvol:	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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