2,2-Bis(fluoromethyl)-1,3-difluoropropane

Inchi: InChI=1S/C5H8F4/c6-1-5(2-7,3-8)4-9/h1-4H2
InchiKey: ACBHFORVXDMTHO-UHFFFAOYSA-N
Formula: C5H8F4
SMILES: FCC(CF)(CF)CF
Mol. weight [g/mol]: 144.11
CAS: 338-23-8

Physical Properties

Property code	Value	Unit	Source
gf	-785.18	kJ/mol	Joback Method
hf	-939.72	kJ/mol	Joback Method
hfus	13.61	kJ/mol	Joback Method
hvap	22.16	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.851		Crippen Method
mcvol	88.390	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
ss	290.16	J/mol×K	NIST Webbook
tb	307.65	K	Joback Method
tc	445.73	K	Joback Method
tf	362.00 ± 1.00	K	NIST Webbook
tt	367.06 ± 0.01	K	NIST Webbook
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.95	J/mol×K	307.65	Joback Method
cpg	165.82	J/mol×K	330.66	Joback Method
cpg	174.33	J/mol×K	353.68	Joback Method
cpg	182.48	J/mol×K	376.69	Joback Method
cpg	190.29	J/mol×K	399.70	Joback Method
cpg	197.76	J/mol×K	422.72	Joback Method
cpg	204.91	J/mol×K	445.73	Joback Method

cps	212.55	J/mol×K	298.15	NIST Webbook
hfust	5.14	kJ/mol	367.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C338238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume