1,3-Butadiene, 2-methyl-3-fluoro

Inchi: InChI=1S/C5H7F/c1-4(2)5(3)6/h1,3H2,2H3
InchiKey: YAYWOMCZHXJZEP-UHFFFAOYSA-N
Formula: C5H7F
SMILES: C=C(C)C(=C)F
Mol. weight [g/mol]: 86.11

Physical Properties

Property code	Value	Unit	Source
gf	-45.01	kJ/mol	Joback Method
hf	-111.36	kJ/mol	Joback Method
hfus	6.61	kJ/mol	Joback Method
hvap	24.73	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.046		Crippen Method
mcvol	74.480	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
rinpol	530.00		NIST Webbook
rinpol	530.00		NIST Webbook
tb	306.19	K	Joback Method
tc	472.78	K	Joback Method
tf	115.26	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	110.10	J/mol×K	306.19	Joback Method
cpg	117.80	J/mol×K	333.95	Joback Method
cpg	125.15	J/mol×K	361.72	Joback Method
cpg	132.17	J/mol×K	389.48	Joback Method
cpg	138.87	J/mol×K	417.25	Joback Method
cpg	145.27	J/mol×K	445.01	Joback Method
cpg	151.36	J/mol×K	472.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R510860&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume