Butane, 1,1,1-trifluoro

Inchi: InChI=1S/C4H7F3/c1-2-3-4(5,6)7/h2-3H2,1H3
InchiKey: LDRPULCXZDDSGE-UHFFFAOYSA-N
Formula: C4H7F3
SMILES: CCCC(F)(F)F
Mol. weight [g/mol]: 112.09

Physical Properties

Property code	Value	Unit	Source
gf	-598.79	kJ/mol	Joback Method
hf	-722.97	kJ/mol	Joback Method
hfus	7.94	kJ/mol	Joback Method
hvap	20.75	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.349		Crippen Method
mcvol	72.530	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	448.00		NIST Webbook
tb	285.50	K	Joback Method
tc	429.82	K	Joback Method
tf	139.03	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.76	J/mol×K	285.50	Joback Method
cpg	125.73	J/mol×K	309.55	Joback Method
cpg	133.35	J/mol×K	333.61	Joback Method
cpg	140.65	J/mol×K	357.66	Joback Method
cpg	147.61	J/mol×K	381.71	Joback Method
cpg	154.26	J/mol×K	405.76	Joback Method
cpg	160.61	J/mol×K	429.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511383&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
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