1-Iodo-2-trifluoromethylpropane

Other names: 1,1,1-Trifluoro-3-iodo-2-methylpropane
Inchi: InChI=1S/C4H6F3I/c1-3(2-8)4(5,6)7/h3H,2H2,1H3
InchiKey: UEEFSGKHKKFYRL-UHFFFAOYSA-N
Formula: C4H6F3I
SMILES: CC(CI)C(F)(F)F
Mol. weight [g/mol]: 237.99
CAS: 26653-47-4

Physical Properties

Property code	Value	Unit	Source
gf	-543.11	kJ/mol	Joback Method
hf	-651.38	kJ/mol	Joback Method
hfus	8.82	kJ/mol	Joback Method
hvap	29.74	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.620		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	378.20	K	Joback Method
tc	566.53	K	Joback Method
tf	182.09	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.64	J/mol×K	378.20	Joback Method
cpg	172.21	J/mol×K	409.59	Joback Method
cpg	180.19	J/mol×K	440.98	Joback Method
cpg	187.63	J/mol×K	472.36	Joback Method
cpg	194.53	J/mol×K	503.75	Joback Method
cpg	200.94	J/mol×K	535.14	Joback Method
cpg	206.89	J/mol×K	566.53	Joback Method
hvapt	30.40	kJ/mol	333.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45084e+01
Coeff. B	-3.65190e+03
Temperature range (K), min.	256.80
Temperature range (K), max.	397.08

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26653474&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume