Butane, 1,1,1,2,2,3,3-heptafluoro-4-iodo-

Other names:	Heptafluorobutyl iodide
	2,2,3,3,4,4,4-Heptafluoro-1-iodobutane
	1H,1H-Heptafluoro-1-iodobutane
	1H,1H-Heptafluorobutyl iodide
	1-Iodo-1H,1H-perfluorobutane
	1,1,1,2,2,3,3-heptafluoro-4-iodobutane
Inchi:	InChI=1S/C4H2F7I/c5-2(6,1-12)3(7,8)4(9,10)11/h1H2
InchiKey:	AFHPVXVEXINDFS-UHFFFAOYSA-N
Formula:	C4H2F7I
SMILES:	FC(F)(F)C(F)(F)C(F)(F)CI
Mol. weight [g/mol]:	309.95
CAS:	374-98-1

Physical Properties

Property code	Value	Unit	Source
gf	-1314.23	kJ/mol	Joback Method
hf	-1448.04	kJ/mol	Joback Method
hfus	9.84	kJ/mol	Joback Method
hvap	24.26	kJ/mol	Joback Method
ie	9.96 ± 0.02	eV	NIST Webbook
log10ws	-3.74		Crippen Method
logp	3.254		Crippen Method
mcvol	105.430	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	369.26	K	Joback Method
tc	536.77	K	Joback Method
tf	204.29	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.37	J/mol×K	369.26	Joback Method
cpg	208.71	J/mol×K	397.18	Joback Method

cpg	217.27	J/mol×K	425.10	Joback Method
cpg	225.07	J/mol×K	453.02	Joback Method
cpg	232.16	J/mol×K	480.94	Joback Method
cpg	238.58	J/mol×K	508.85	Joback Method
cpg	244.38	J/mol×K	536.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.30 ± 0.30	K	98.70	NIST Webbook

Sources

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=C374981&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume