(S)-(+)-1-Iodo-2-methylbutane

Inchi: InChI=1S/C5H11I/c1-3-5(2)4-6/h5H,3-4H2,1-2H3/t5-/m1/s1
InchiKey: RHBHXHXNWHTGSO-RXMQYKEDSA-N
Formula: C5H11I
SMILES: CCC(C)CI
Mol. weight [g/mol]: 198.05
CAS: 29394-58-9

Physical Properties

Property code	Value	Unit	Source
gf	46.90	kJ/mol	Joback Method
hf	-74.94	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.468		Crippen Method
mcvol	107.130	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	421.20	K	NIST Webbook
tc	613.94	K	Joback Method
tf	189.17	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.15	J/mol×K	406.50	Joback Method
cpg	182.14	J/mol×K	441.07	Joback Method
cpg	191.61	J/mol×K	475.65	Joback Method
cpg	200.59	J/mol×K	510.22	Joback Method
cpg	209.09	J/mol×K	544.79	Joback Method
cpg	217.13	J/mol×K	579.36	Joback Method
cpg	224.75	J/mol×K	613.94	Joback Method
dvisc	0.0102765	Pa×s	189.17	Joback Method
dvisc	0.0037890	Pa×s	225.39	Joback Method

dvisc	0.0018416	Pa×s	261.61	Joback Method
dvisc	0.0010668	Pa×s	297.84	Joback Method
dvisc	0.0006956	Pa×s	334.06	Joback Method
dvisc	0.0004932	Pa×s	370.28	Joback Method
dvisc	0.0003718	Pa×s	406.50	Joback Method

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=C29394589&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume