

1,2,4-Trichloro-3-iodobutane

Inchi:	InChI=1S/C4H6Cl3I/c5-1-3(7)4(8)2-6/h3-4H,1-2H2
InchiKey:	KCMZWZSUXFIJLT-UHFFFAOYSA-N
Formula:	C4H6Cl3I
SMILES:	CICC(Cl)C(I)CCI
Mol. weight [g/mol]:	287.35
CAS:	116401-08-2

Physical Properties

Property code	Value	Unit	Source
gf	0.25	kJ/mol	Joback Method
hf	-106.80	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	46.25	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.875		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
tb	495.47	K	Joback Method
tc	731.61	K	Joback Method
tf	252.66	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.98	J/molxK	495.47	Joback Method
cpg	207.19	J/molxK	534.83	Joback Method
cpg	213.85	J/molxK	574.18	Joback Method
cpg	220.00	J/molxK	613.54	Joback Method
cpg	225.66	J/molxK	652.90	Joback Method
cpg	230.89	J/molxK	692.26	Joback Method
cpg	235.71	J/molxK	731.61	Joback Method
dvisc	0.0084667	Paxs	252.66	Joback Method
dvisc	0.0034707	Paxs	293.13	Joback Method

dvisc	0.0017663	Paxs	333.60	Joback Method
dvisc	0.0010404	Paxs	374.07	Joback Method
dvisc	0.0006795	Paxs	414.53	Joback Method
dvisc	0.0004788	Paxs	455.00	Joback Method
dvisc	0.0003572	Paxs	495.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C116401082&Units=SI

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

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