

isopropyl thiobutyrate

Inchi:	InChI=1S/C7H14OS/c1-4-5-7(8)9-6(2)3/h6H,4-5H2,1-3H3
InchiKey:	QWILNQBBMPJVDW-UHFFFAOYSA-N
Formula:	C7H14OS
SMILES:	CCCC(=O)SC(C)C
Mol. weight [g/mol]:	146.25

Physical Properties

Property code	Value	Unit	Source
gf	-90.18	kJ/mol	Joback Method
hf	-263.80	kJ/mol	Joback Method
hfus	16.09	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.455		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
tb	481.77	K	Joback Method
tc	684.48	K	Joback Method
tf	237.98	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.67	J/molxK	481.77	Joback Method
cpg	277.06	J/molxK	515.56	Joback Method
cpg	288.88	J/molxK	549.34	Joback Method
cpg	300.15	J/molxK	583.13	Joback Method
cpg	310.87	J/molxK	616.91	Joback Method
cpg	321.06	J/molxK	650.70	Joback Method
cpg	330.71	J/molxK	684.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R148391&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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