isobutyl thiobutyrate

Inchi: InChI=1S/C8H16OS/c1-4-5-8(9)10-6-7(2)3/h7H,4-6H2,1-3H3
InchiKey: DUODPBLEEBFAEG-UHFFFAOYSA-N
Formula: C8H16OS
SMILES: CCCC(=O)SCC(C)C
Mol. weight [g/mol]: 160.28

Physical Properties

Property code	Value	Unit	Source
gf	-81.76	kJ/mol	Joback Method
hf	-284.44	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.702		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
tb	504.65	K	Joback Method
tc	704.63	K	Joback Method
tf	249.25	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.83	J/mol×K	504.65	Joback Method
cpg	321.28	J/mol×K	537.98	Joback Method
cpg	334.10	J/mol×K	571.31	Joback Method
cpg	346.32	J/mol×K	604.64	Joback Method
cpg	357.93	J/mol×K	637.97	Joback Method
cpg	368.95	J/mol×K	671.30	Joback Method
cpg	379.39	J/mol×K	704.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R148371&Units=SI
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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