Propanethioic acid, S-(2-methylpropyl) ester

Other names: Propionic acid, thio-, S-isobutyl ester
Inchi: InChI=1S/C7H14OS/c1-4-7(8)9-5-6(2)3/h6H,4-5H2,1-3H3
InchiKey: WFEQYXZOOLMWEM-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCC(=O)SCC(C)C
Mol. weight [g/mol]: 146.25
CAS: 2432-48-6

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	-2.17		Crippen Method
logp	2.312		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1002.00		NIST Webbook
rinpol	1002.00		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/mol×K	481.77	Joback Method
cpg	277.06	J/mol×K	515.56	Joback Method
cpg	288.88	J/mol×K	549.34	Joback Method
cpg	300.15	J/mol×K	583.13	Joback Method
cpg	310.87	J/mol×K	616.91	Joback Method
cpg	321.06	J/mol×K	650.70	Joback Method

cpg	330.71	J/mol×K	684.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432486&Units=SI

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