2-(Isopropyldisulfanyl)butane

Other names: 2,5-dimethyl-3,4-dithiaheptane
Inchi: InChI=1S/C7H16S2/c1-5-7(4)9-8-6(2)3/h6-7H,5H2,1-4H3
InchiKey: GWDWLWHLJNZIBY-UHFFFAOYSA-N
Formula: C7H16S2
SMILES: CCC(C)SSC(C)C
Mol. weight [g/mol]: 164.33
CAS: 67421-86-7

Physical Properties

Property code	Value	Unit	Source
gf	69.42	kJ/mol	Joback Method
hf	-114.63	kJ/mol	Joback Method
hfus	15.10	kJ/mol	Joback Method
hvap	44.03	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.575		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1119.00		NIST Webbook
rinpol	1119.00		NIST Webbook
tb	496.24	K	Joback Method
tc	715.16	K	Joback Method
tf	207.45	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.83	J/mol×K	496.24	Joback Method
cpg	311.09	J/mol×K	532.73	Joback Method
cpg	324.67	J/mol×K	569.21	Joback Method
cpg	337.56	J/mol×K	605.70	Joback Method
cpg	349.78	J/mol×K	642.19	Joback Method
cpg	361.33	J/mol×K	678.67	Joback Method

cpg	372.21	J/mol×K	715.16	Joback Method

Sources

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=C67421867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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