3-ethyl-2,4-dithiapentane

Inchi: InChI=1S/C5H12S2/c1-4-5(6-2)7-3/h5H,4H2,1-3H3
InchiKey: VKKDPAMHYXBCEE-UHFFFAOYSA-N
Formula: C5H12S2
SMILES: CCC(SC)SC
Mol. weight [g/mol]: 136.28

Physical Properties

Property code	Value	Unit	Source
gf	55.02	kJ/mol	Joback Method
hf	-68.07	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	39.97	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.449		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
tb	450.92	K	Joback Method
tc	671.44	K	Joback Method
tf	199.91	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.94	J/mol×K	450.92	Joback Method
cpg	225.27	J/mol×K	487.67	Joback Method
cpg	236.10	J/mol×K	524.43	Joback Method
cpg	246.44	J/mol×K	561.18	Joback Method
cpg	256.29	J/mol×K	597.94	Joback Method
cpg	265.64	J/mol×K	634.69	Joback Method
cpg	274.48	J/mol×K	671.44	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=R156639&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