6-Ethyl-4,5,7-trithia-2,8-decadiene

Inchi: InChI=1S/C9H16S3/c1-4-7-10-9(6-3)12-11-8-5-2/h4-5,7-9H,6H2,1-3H3/b7-4+,8-5+
InchiKey: YFTPKQUIYROJDX-NSLJXJERSA-N
Formula: C9H16S3
SMILES: CC=CSSC(CC)SC=CC
Mol. weight [g/mol]: 220.42
CAS: 126876-28-6

Physical Properties

Property code	Value	Unit	Source
gf	282.26	kJ/mol	Joback Method
hf	125.68	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	55.61	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.904		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1603.10		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1547.60		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1547.60		NIST Webbook
rinpol	1603.10		NIST Webbook
tb	619.54	K	Joback Method
tc	865.36	K	Joback Method
tf	269.23	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.05	J/mol×K	619.54	Joback Method
cpg	415.78	J/mol×K	660.51	Joback Method
cpg	429.49	J/mol×K	701.48	Joback Method
cpg	442.22	J/mol×K	742.45	Joback Method
cpg	454.03	J/mol×K	783.42	Joback Method
cpg	464.95	J/mol×K	824.39	Joback Method
cpg	475.03	J/mol×K	865.36	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=C126876286&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

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