3,5-dithianonane

Inchi: InChI=1S/C7H16S2/c1-3-5-6-9-7-8-4-2/h3-7H2,1-2H3
InchiKey: OXKJXXJWXSXRDM-UHFFFAOYSA-N
Formula: C7H16S2
SMILES: CCCCSCSCC
Mol. weight [g/mol]: 164.33
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	74.30	kJ/mol	Joback Method
hf	-104.07	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.230		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1239.00		NIST Webbook
rinpol	1239.00		NIST Webbook
tb	497.12	K	Joback Method
tc	706.23	K	Joback Method
tf	237.45	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.36	J/mol×K	497.12	Joback Method
cpg	309.83	J/mol×K	531.97	Joback Method
cpg	322.69	J/mol×K	566.82	Joback Method
cpg	334.95	J/mol×K	601.67	Joback Method
cpg	346.61	J/mol×K	636.52	Joback Method
cpg	357.67	J/mol×K	671.38	Joback Method
cpg	368.15	J/mol×K	706.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60986e+01
Coeff. B	-4.64732e+03
Coeff. C	-8.01920e+01
Temperature range (K), min.	374.12
Temperature range (K), max.	511.01

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=R156535&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume