2,4-dithiaoctane

Inchi: InChI=1S/C6H14S2/c1-3-4-5-8-6-7-2/h3-6H2,1-2H3
InchiKey: YCAQLLUVGIOAHA-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CCCCSCSC
Mol. weight [g/mol]: 150.31
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	65.88	kJ/mol	Joback Method
hf	-83.43	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	42.58	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.840		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
tb	474.24	K	Joback Method
tc	686.46	K	Joback Method
tf	226.18	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.01	J/mol×K	474.24	Joback Method
cpg	266.31	J/mol×K	509.61	Joback Method
cpg	278.07	J/mol×K	544.98	Joback Method
cpg	289.29	J/mol×K	580.35	Joback Method
cpg	299.98	J/mol×K	615.72	Joback Method
cpg	310.13	J/mol×K	651.09	Joback Method
cpg	319.76	J/mol×K	686.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64270e+01
Coeff. B	-4.60060e+03
Coeff. C	-7.54660e+01
Temperature range (K), min.	360.52
Temperature range (K), max.	489.36

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=R155676&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