

3,5-dithiaoctane

Inchi: InChI=1S/C6H14S2/c1-3-5-8-6-7-4-2/h3-6H2,1-2H3
InchiKey: RTXKOZHNOGUZNW-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CCCSCSCC
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	1144.00		NIST Webbook
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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/molxK	474.24	Joback Method
cpg	266.31	J/molxK	509.61	Joback Method
cpg	278.07	J/molxK	544.98	Joback Method
cpg	289.29	J/molxK	580.35	Joback Method
cpg	299.98	J/molxK	615.72	Joback Method
cpg	310.13	J/molxK	651.09	Joback Method
cpg	319.76	J/molxK	686.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60134e+01
Coeff. B	-4.45152e+03
Coeff. C	-7.44090e+01
Temperature range (K), min.	357.48
Temperature range (K), max.	490.36

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R156540&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
hvac:	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

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