

1,10-Decanedithiol

Other names:	1,10-Dimercaptodecane decane-1,10-dithiol
Inchi:	InChI=1S/C10H22S2/c11-9-7-5-3-1-2-4-6-8-10-12/h11-12H,1-10H2
InchiKey:	UOQACRNTVQWTFE-UHFFFAOYSA-N
Formula:	C10H22S2
SMILES:	SCCCCCCCCCCS
Mol. weight [g/mol]:	206.41
CAS:	1191-67-9

Physical Properties

Property code	Value	Unit	Source
gf	92.10	kJ/mol	Joback Method
hf	-172.77	kJ/mol	Joback Method
hfus	29.74	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.967		Crippen Method
mvol	184.460	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	553.92	K	Joback Method
tc	754.39	K	Joback Method
tf	275.38	K	Joback Method
vc	0.704	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.02	J/molxK	553.92	Joback Method
cpg	445.05	J/molxK	587.33	Joback Method
cpg	460.29	J/molxK	620.74	Joback Method
cpg	474.77	J/molxK	654.15	Joback Method
cpg	488.50	J/molxK	687.56	Joback Method
cpg	501.52	J/molxK	720.98	Joback Method
cpg	513.85	J/molxK	754.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35394e+01
Coeff. B	-4.36204e+03
Coeff. C	-9.94900e+01
Temperature range (K), min.	428.65
Temperature range (K), max.	629.64

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=C1191679&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure

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

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