

5-methyl-3-thiadecane

Inchi:	InChI=1S/C10H22S/c1-4-6-7-8-10(3)9-11-5-2/h10H,4-9H2,1-3H3
InchiKey:	ZRITYAYIKDALFO-UHFFFAOYSA-N
Formula:	C10H22S
SMILES:	CCCCC(C)CSCC
Mol. weight [g/mol]:	174.35
CAS:	---

Physical Properties

Property code	Value	Unit	Source
gf	64.00	kJ/mol	Joback Method
hf	-213.14	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.956		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1216.00		NIST Webbook
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tb	496.54	K	Joback Method
tc	682.34	K	Joback Method
tf	221.86	K	Joback Method
vc	0.643	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.11	J/mol×K	496.54	Joback Method
cpg	392.28	J/mol×K	527.51	Joback Method
cpg	407.76	J/mol×K	558.47	Joback Method
cpg	422.57	J/mol×K	589.44	Joback Method
cpg	436.72	J/mol×K	620.41	Joback Method
cpg	450.23	J/mol×K	651.37	Joback Method
cpg	463.12	J/mol×K	682.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53810e+01
Coeff. B	-4.41450e+03
Coeff. C	-7.83540e+01
Temperature range (K), min.	370.83
Temperature range (K), max.	516.75

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=R157429&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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