

1-Eicosanethiol

Inchi:	InChI=1S/C20H42S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h21H,2-20
InchiKey:	YYHYWOPDNMFEAV-UHFFFAOYSA-N
Formula:	C20H42S
SMILES:	CCCCCCCCCCCCCCCCCCCCCS
Mol. weight [g/mol]:	314.61
CAS:	13373-97-2

Physical Properties

Property code	Value	Unit	Source
gf	146.91	kJ/mol	Joback Method
hf	-417.65	kJ/mol	Joback Method
hfus	51.60	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.958		Crippen Method
mcvol	309.010	ml/mol	McGowan Method
pc	1058.26	kPa	Joback Method
tb	719.86	K	Joback Method
tc	893.65	K	Joback Method
tf	311.15 ± 1.00	K	NIST Webbook
vc	1.210	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.35	J/mol×K	719.86	Joback Method
cpg	933.95	J/mol×K	748.83	Joback Method
cpg	953.61	J/mol×K	777.79	Joback Method
cpg	972.35	J/mol×K	806.76	Joback Method
cpg	990.21	J/mol×K	835.72	Joback Method
cpg	1007.23	J/mol×K	864.69	Joback Method
cpg	1023.43	J/mol×K	893.65	Joback Method
cpl	725.84	J/mol×K	300.00	NIST Webbook
hvapt	81.30	kJ/mol	603.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54895e+01
Coeff. B	-5.80358e+03
Coeff. C	-1.23562e+02
Temperature range (K), min.	505.33
Temperature range (K), max.	693.77

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13373972&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

Legend

cp_g:	Ideal gas heat capacity
cp_l:	Liquid phase 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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_cvol:	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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