1-Docosanethiol

Inchi: InChI=1S/C22H46S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23/h23
InchiKey: NNZMLOHQRXHPOZ-UHFFFAOYSA-N
Formula: C22H46S
SMILES: CCCCCCCCCCCCCCCCCCCCCCS
Mol. weight [g/mol]: 342.67
CAS: 7773-83-3

Physical Properties

Property code	Value	Unit	Source
gf	163.75	kJ/mol	Joback Method
hf	-458.93	kJ/mol	Joback Method
hfus	56.78	kJ/mol	Joback Method
hvap	71.30	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.738		Crippen Method
mcvol	337.190	ml/mol	McGowan Method
pc	937.49	kPa	Joback Method
tb	765.62	K	Joback Method
tc	942.73	K	Joback Method
tf	315.90 ± 1.00	K	NIST Webbook
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.02	J/mol×K	765.62	Joback Method
cpg	1057.38	J/mol×K	795.14	Joback Method
cpg	1077.72	J/mol×K	824.66	Joback Method
cpg	1097.08	J/mol×K	854.18	Joback Method
cpg	1115.50	J/mol×K	883.70	Joback Method
cpg	1133.02	J/mol×K	913.21	Joback Method
cpg	1149.68	J/mol×K	942.73	Joback Method
hvapt	107.70	kJ/mol	558.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55097e+01
Coeff. B	-6.00126e+03
Coeff. C	-1.30209e+02
Temperature range (K), min.	524.45
Temperature range (K), max.	718.67

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7773833&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/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

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