

Tert-octyl mercaptan

Inchi:	InChI=1S/C8H18S/c1-8(2,3)6-4-5-7-9/h9H,4-7H2,1-3H3
InchiKey:	YBZXKSZKVDFBJI-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CC(C)(C)CCCCS
Mol. weight [g/mol]:	146.29
CAS:	7341-16-4

Physical Properties

Property code	Value	Unit	Source
gf	48.71	kJ/mol	Joback Method
hf	-178.72	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	38.84	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.133		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	2761.36	kPa	Joback Method
tb	442.07	K	Joback Method
tc	639.83	K	Joback Method
tf	218.80	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.00	J/mol×K	442.07	Joback Method
cpg	302.27	J/mol×K	475.03	Joback Method
cpg	316.73	J/mol×K	507.99	Joback Method
cpg	330.41	J/mol×K	540.95	Joback Method
cpg	343.35	J/mol×K	573.91	Joback Method
cpg	355.57	J/mol×K	606.87	Joback Method
cpg	367.11	J/mol×K	639.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.24305e+01
Coeff. B	-3.19364e+03
Coeff. C	-6.03150e+01
Temperature range (K), min.	323.32
Temperature range (K), max.	508.92

Sources

KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1842
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7341164&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.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp _g :	Ideal gas heat capacity
g _f :	Standard Gibbs free energy of formation
h _f :	Enthalpy of formation at standard conditions
h _{fus} :	Enthalpy of fusion at standard conditions
h _{vap} :	Enthalpy of vaporization at standard conditions
log ₁₀ ws:	Log ₁₀ of Water solubility in mol/l
log _p :	Octanol/Water partition coefficient
mc _{vol} :	McGowan's characteristic volume
nf _{paf} :	NFPA Fire Rating
nf _{pah} :	NFPA Health Rating
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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