

3-Heptyne, 7-chloro-

Other names:	7-Chloro-3-heptyne
Inchi:	InChI=1S/C7H11Cl/c1-2-3-4-5-6-7-8/h2,5-7H2,1H3
InchiKey:	NFSWUGZOVBYRKR-UHFFFAOYSA-N
Formula:	C7H11Cl
SMILES:	CCC#CCCCCl
Mol. weight [g/mol]:	130.62
CAS:	51575-85-0

Physical Properties

Property code	Value	Unit	Source
gf	198.93	kJ/mol	Joback Method
hf	68.75	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	37.71	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.419		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	405.99	K	Joback Method
tc	602.63	K	Joback Method
tf	304.67	K	Joback Method
vc	0.439	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.45	J/mol×K	405.99	Joback Method
cpg	207.84	J/mol×K	438.76	Joback Method
cpg	217.79	J/mol×K	471.54	Joback Method
cpg	227.31	J/mol×K	504.31	Joback Method
cpg	236.41	J/mol×K	537.08	Joback Method
cpg	245.10	J/mol×K	569.86	Joback Method
cpg	253.40	J/mol×K	602.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34177e+01
Coeff. B	-3.51943e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	330.72
Temperature range (K), max.	496.84

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51575850&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
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
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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