

6-Tridecanone

Other names:	n-Amyl n-heptyl ketone tridecan-6-one
Inchi:	InChI=1S/C13H26O/c1-3-5-7-8-10-12-13(14)11-9-6-4-2/h3-12H2,1-2H3
InchiKey:	KPVFRXPKBAAIIE-UHFFFAOYSA-N
Formula:	C13H26O
SMILES:	CCCCCCCC(=O)CCCC
Mol. weight [g/mol]:	198.34
CAS:	22026-12-6

Physical Properties

Property code	Value	Unit	Source
gf	-70.34	kJ/mol	Joback Method
hf	-424.23	kJ/mol	Joback Method
hfus	31.02	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.496		Crippen Method
mvol	195.600	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rhoc	240.00 ± 7.93	kg/m3	NIST Webbook
tb	550.71	K	Joback Method
tc	709.30 ± 2.70	K	NIST Webbook
tf	286.20	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.12	J/molxK	550.71	Joback Method
cpg	502.70	J/molxK	578.88	Joback Method
cpg	518.60	J/molxK	607.06	Joback Method
cpg	533.84	J/molxK	635.23	Joback Method
cpg	548.43	J/molxK	663.40	Joback Method
cpg	562.38	J/molxK	691.58	Joback Method

cpg	575.73	J/mol×K	719.75	Joback Method
dvisc	0.0042194	Paxs	286.20	Joback Method
dvisc	0.0018390	Paxs	330.28	Joback Method
dvisc	0.0009747	Paxs	374.37	Joback Method
dvisc	0.0005905	Paxs	418.46	Joback Method
dvisc	0.0003936	Paxs	462.54	Joback Method
dvisc	0.0002816	Paxs	506.62	Joback Method
dvisc	0.0002125	Paxs	550.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52310e+01
Coeff. B	-4.71493e+03
Coeff. C	-8.95600e+01
Temperature range (K), min.	405.08
Temperature range (K), max.	564.88

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22026126&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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