

13-Methyltetradecanal

Inchi:	InChI=1S/C15H30O/c1-15(2)13-11-9-7-5-3-4-6-8-10-12-14-16/h14-15H,3-13H2,1-2H3
InchiKey:	KEKMLOYOUUVRDN-UHFFFAOYSA-N
Formula:	C15H30O
SMILES:	CC(C)CCCCCCCCCCC=O
Mol. weight [g/mol]:	226.40
CAS:	75853-51-9

Physical Properties

Property code	Value	Unit	Source
gf	-26.54	kJ/mol	Joback Method
hf	-443.79	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	5.132		Crippen Method
mcvol	223.780	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
rinpol	1680.30		NIST Webbook
rinpol	1680.30		NIST Webbook
tb	590.82	K	Joback Method
tc	757.55	K	Joback Method
tf	285.81	K	Joback Method
vc	0.886	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.34	J/mol×K	590.82	Joback Method
cpg	671.53	J/mol×K	729.77	Joback Method
cpg	656.70	J/mol×K	701.98	Joback Method
cpg	641.18	J/mol×K	674.19	Joback Method
cpg	624.97	J/mol×K	646.40	Joback Method
cpg	608.03	J/mol×K	618.61	Joback Method
cpg	685.70	J/mol×K	757.55	Joback Method

dvisc	0.0001793	Paxs	590.82	Joback Method
dvisc	0.0002447	Paxs	539.98	Joback Method
dvisc	0.0003564	Paxs	489.15	Joback Method
dvisc	0.0005663	Paxs	438.31	Joback Method
dvisc	0.0010162	Paxs	387.48	Joback Method
dvisc	0.0021756	Paxs	336.64	Joback Method
dvisc	0.0061062	Paxs	285.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51918e+01
Coeff. B	-5.00182e+03
Coeff. C	-9.81230e+01
Temperature range (K), min.	433.72
Temperature range (K), max.	604.36

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75853519&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/79-335-3/13-Methyltetradecanal.pdf>

Generated by Cheméo on 2024-04-19 22:12:15.272623471 +0000 UTC m=+15853984.193200783.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.