

3-Ethyl-3-methyltridecane

Inchi:	InChI=1S/C16H34/c1-5-8-9-10-11-12-13-14-15-16(4,6-2)7-3/h5-15H2,1-4H3
InchiKey:	FPUUAPQHIFZHQCQ-UHFFFAOYSA-N
Formula:	C16H34
SMILES:	CCCCCCCCC(C)(CC)CC
Mol. weight [g/mol]:	226.44

Physical Properties

Property code	Value	Unit	Source
gf	86.68	kJ/mol	Joback Method
hf	-382.32	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	49.91	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.344		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinsol	1549.00		NIST Webbook
tb	562.25	K	Joback Method
tc	728.23	K	Joback Method
tf	272.50	K	Joback Method
vc	0.920	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.09	J/molxK	562.25	Joback Method
cpg	634.19	J/molxK	589.91	Joback Method
cpg	653.40	J/molxK	617.58	Joback Method
cpg	671.77	J/molxK	645.24	Joback Method
cpg	689.32	J/molxK	672.91	Joback Method
cpg	706.10	J/molxK	700.57	Joback Method
cpg	722.12	J/molxK	728.23	Joback Method
dvisc	0.0068269	Paxs	272.50	Joback Method
dvisc	0.0021907	Paxs	320.79	Joback Method

dvisc	0.0009465	Paxs	369.08	Joback Method
dvisc	0.0004966	Paxs	417.38	Joback Method
dvisc	0.0002978	Paxs	465.67	Joback Method
dvisc	0.0001966	Paxs	513.96	Joback Method
dvisc	0.0001394	Paxs	562.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R415379&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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