

3-Ethyl-3-methyl-pentacosane

Inchi:	InChI=1S/C28H58/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28
InchiKey:	DPYKIUKBORPTNH-UHFFFAOYSA-N
Formula:	C28H58
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)(CC)CC
Mol. weight [g/mol]:	394.76

Physical Properties

Property code	Value	Unit	Source
gf	187.72	kJ/mol	Joback Method
hf	-630.00	kJ/mol	Joback Method
hfus	60.86	kJ/mol	Joback Method
hvap	76.63	kJ/mol	Joback Method
log10ws	-11.30		Crippen Method
logp	11.025		Crippen Method
mcvol	405.380	ml/mol	McGowan Method
pc	661.87	kPa	Joback Method
tb	836.81	K	Joback Method
tc	1024.78	K	Joback Method
tf	407.74	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.95	J/molxK	836.81	Joback Method
cpg	1372.99	J/molxK	868.14	Joback Method
cpg	1396.76	J/molxK	899.47	Joback Method
cpg	1419.34	J/molxK	930.80	Joback Method
cpg	1440.80	J/molxK	962.13	Joback Method
cpg	1461.21	J/molxK	993.45	Joback Method
cpg	1480.64	J/molxK	1024.78	Joback Method
dvisc	0.0014268	Paxs	407.74	Joback Method
dvisc	0.0004444	Paxs	479.25	Joback Method
dvisc	0.0001874	Paxs	550.76	Joback Method

dvisc	0.0000964	Paxs	622.27	Joback Method
dvisc	0.0000568	Paxs	693.79	Joback Method
dvisc	0.0000370	Paxs	765.30	Joback Method
dvisc	0.0000259	Paxs	836.81	Joback Method

Sources

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=R415344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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