

11-methyl-heptatriacontane

Inchi:	InChI=1S/C38H78/c1-4-6-8-10-12-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-3
InchiKey:	YCCALXWXVZUPJR-UHFFFAOYSA-N
Formula:	C38H78
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCC
Mol. weight [g/mol]:	535.03

Physical Properties

Property code	Value	Unit	Source
gf	266.64	kJ/mol	Joback Method
hf	-832.93	kJ/mol	Joback Method
hfus	90.65	kJ/mol	Joback Method
hvap	99.79	kJ/mol	Joback Method
log10ws	-15.49		Crippen Method
logp	14.926		Crippen Method
mcvol	546.280	ml/mol	McGowan Method
pc	423.73	kPa	Joback Method
rinpol	3735.00		NIST Webbook
rinpol	3735.00		NIST Webbook
rinpol	3722.00		NIST Webbook
rinpol	3735.00		NIST Webbook
rinpol	3722.00		NIST Webbook
tb	1068.40	K	Joback Method
tc	1389.46	K	Joback Method
tf	503.02	K	Joback Method
vc	2.158	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2035.08	J/molxK	1068.40	Joback Method
cpg	2073.73	J/molxK	1121.91	Joback Method
cpg	2109.16	J/molxK	1175.42	Joback Method
cpg	2141.75	J/molxK	1228.93	Joback Method
cpg	2171.93	J/molxK	1282.44	Joback Method

cpg	2200.09	J/mol×K	1335.95	Joback Method
cpg	2226.65	J/mol×K	1389.46	Joback Method
dvisc	0.0003897	Paxs	503.02	Joback Method
dvisc	0.0001137	Paxs	597.25	Joback Method
dvisc	0.0000464	Paxs	691.48	Joback Method
dvisc	0.0000235	Paxs	785.71	Joback Method
dvisc	0.0000138	Paxs	879.94	Joback Method
dvisc	0.0000089	Paxs	974.17	Joback Method
dvisc	0.0000063	Paxs	1068.40	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=R271951&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
mccvol:	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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