3-methyl-triacontane

Inchi:	InChI=1S/C31H64/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-2
InchiKey:	NXCMTLDSKYDELZ-UHFFFAOYSA-N
Formula:	C31H64
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CC
Mol. weight [g/mol]:	436.84
CAS:	72227-01-1

Physical Properties

Property code	Value	Unit	Source
gf	207.70	kJ/mol	Joback Method
hf	-688.45	kJ/mol	Joback Method
hfus	72.52	kJ/mol	Joback Method
hvap	84.21	kJ/mol	Joback Method
log10ws	-12.56		Crippen Method
logp	12.195		Crippen Method
mcvol	447.650	ml/mol	McGowan Method
pc	570.69	kPa	Joback Method
rinpol	3078.00		NIST Webbook
rinpol	3078.00		NIST Webbook
rinpol	3075.00		NIST Webbook
rinpol	3064.00		NIST Webbook
rinpol	3066.00		NIST Webbook
rinpol	3075.00		NIST Webbook
rinpol	3072.90		NIST Webbook
rinpol	3078.00		NIST Webbook
tb	908.24	K	Joback Method
tc	1122.22	K	Joback Method
tf	424.13	K	Joback Method
vc	1.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1550.16	J/mol×K	908.24	Joback Method

cpg	1578.28	J/mol×K	943.90	Joback Method
cpg	1604.74	J/mol×K	979.57	Joback Method
cpg	1629.63	J/mol×K	1015.23	Joback Method
cpg	1653.05	J/mol×K	1050.89	Joback Method
cpg	1675.10	J/mol×K	1086.56	Joback Method
cpg	1695.88	J/mol×K	1122.22	Joback Method
dvisc	0.0011568	Pa×s	424.13	Joback Method
dvisc	0.0003377	Pa×s	504.81	Joback Method
dvisc	0.0001384	Pa×s	585.50	Joback Method
dvisc	0.0000704	Pa×s	666.18	Joback Method
dvisc	0.0000415	Pa×s	746.87	Joback Method
dvisc	0.0000271	Pa×s	827.56	Joback Method
dvisc	0.0000191	Pa×s	908.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72227011&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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