

Pentatriacontane, 3,7-dimethyl

Inchi: InChI=1S/C37H76/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-
InchiKey: VGPJDHPPCZZNLD-UHFFFAOYSA-N
Formula: C37H76
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CC
Mol. weight [g/mol]: 521.01

Physical Properties

Property code	Value	Unit	Source
af	1.3733		Cheméo Relay (1.0)
gf	255.78	kJ/mol	Joback Method
hf	-840.27	kJ/mol	Cheméo Relay (1.0)
hfus	84.54	kJ/mol	Joback Method
hvap	173.48	kJ/mol	Cheméo Relay (1.0)
ie	10.23	eV	Cheméo Relay (1.0)
log10ws	-13.12		Cheméo Relay (1.0)
logp	14.391		Crippen Method
mcvol	532.190	ml/mol	McGowan Method
pc	442.47	kPa	Joback Method
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook
tb	685.53	K	Cheméo Relay (1.0)
tc	852.79	K	Cheméo Relay (1.0)
tf	299.80	K	Cheméo Relay (1.0)
vc	2.075	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1965.02	J/mol×K	1045.08	Joback Method
cpg	2001.02	J/mol×K	1094.29	Joback Method
cpg	2034.16	J/mol×K	1143.50	Joback Method

cpg	2064.75	J/mol×K	1192.71	Joback Method
cpg	2093.10	J/mol×K	1241.92	Joback Method
cpg	2119.51	J/mol×K	1291.13	Joback Method
cpg	2144.28	J/mol×K	1340.34	Joback Method
dvisc	0.0005532	Pa×s	476.75	Joback Method
dvisc	0.0001441	Pa×s	571.47	Joback Method
dvisc	0.0000550	Pa×s	666.19	Joback Method
dvisc	0.0000267	Pa×s	760.91	Joback Method
dvisc	0.0000152	Pa×s	855.64	Joback Method
dvisc	0.0000097	Pa×s	950.36	Joback Method
dvisc	0.0000067	Pa×s	1045.08	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R272409&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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