Pentatriacontane, 5,9-dimethyl

Inchi: InChI=1S/C37H76/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28
InchiKey: AWMCNBMLCHKBNO-UHFFFAOYSA-N
Formula: C37H76
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC(C)CCCC
Mol. weight [g/mol]: 521.01

Physical Properties

Property code	Value	Unit	Source
af	1.3709		Cheméo Relay (1.0)
gf	255.78	kJ/mol	Joback Method
hf	-838.97	kJ/mol	Cheméo Relay (1.0)
hfus	84.54	kJ/mol	Joback Method
hvap	173.78	kJ/mol	Cheméo Relay (1.0)
ie	10.16	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	3580.00		NIST Webbook
rinpol	3578.00		NIST Webbook
rinpol	3580.00		NIST Webbook
rinpol	3580.00		NIST Webbook
tb	683.87	K	Cheméo Relay (1.0)
tc	852.39	K	Cheméo Relay (1.0)
tf	294.88	K	Cheméo Relay (1.0)
vc	2.076	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	2144.28	J/mol×K	1340.34	Joback Method
cpg	2119.51	J/mol×K	1291.13	Joback Method
cpg	2093.10	J/mol×K	1241.92	Joback Method

cpg	2064.75	J/mol×K	1192.71	Joback Method
cpg	2034.16	J/mol×K	1143.50	Joback Method
cpg	2001.02	J/mol×K	1094.29	Joback Method
dvisc	0.0000267	Pa×s	760.91	Joback Method
dvisc	0.0000067	Pa×s	1045.08	Joback Method
dvisc	0.0000097	Pa×s	950.36	Joback Method
dvisc	0.0000152	Pa×s	855.64	Joback Method
dvisc	0.0005532	Pa×s	476.75	Joback Method
dvisc	0.0000550	Pa×s	666.19	Joback Method
dvisc	0.0001441	Pa×s	571.47	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R418110&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

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