4-Methylheneicosane

Other names: 4-methylheneicosane
Inchi: InChI=1S/C22H46/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-22(3)20-5-2/h22H,4-
InchiKey: DOVNYJDAQVFZKC-UHFFFAOYSA-N
Formula: C22H46
SMILES: CCCCCCCCCCCCCCCCCC(C)CCC
Mol. weight [g/mol]: 310.60
CAS: 25117-29-7

Physical Properties

Property code	Value	Unit	Source
af	0.8853		Cheméo Relay (1.0)
gf	131.92	kJ/mol	Joback Method
hf	-505.76	kJ/mol	Cheméo Relay (1.0)
hfus	49.21	kJ/mol	Joback Method
hvap	106.74	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
log10ws	-9.12		Cheméo Relay (1.0)
logp	8.684		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
tb	587.95	K	Cheméo Relay (1.0)
tc	759.28	K	Cheméo Relay (1.0)
tf	281.97	K	Cheméo Relay (1.0)
vc	1.265	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.39	J/mol×K	702.32	Joback Method
cpg	984.38	J/mol×K	729.81	Joback Method
cpg	1005.42	J/mol×K	757.30	Joback Method
cpg	1025.55	J/mol×K	784.79	Joback Method
cpg	1044.78	J/mol×K	812.28	Joback Method
cpg	1063.16	J/mol×K	839.77	Joback Method

cpg	1080.72	J/mol×K	867.26	Joback Method
dvisc	0.0040182	Pa×s	322.70	Joback Method
dvisc	0.0011754	Pa×s	385.97	Joback Method
dvisc	0.0004861	Pa×s	449.24	Joback Method
dvisc	0.0002500	Pa×s	512.51	Joback Method
dvisc	0.0001488	Pa×s	575.78	Joback Method
dvisc	0.0000982	Pa×s	639.05	Joback Method
dvisc	0.0000698	Pa×s	702.32	Joback Method
hvapt	70.90	kJ/mol	564.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C25117297&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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