2-methyl-1-eicosene

Inchi: InChI=1S/C21H42/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(2)3/h2,4-20H2,1

InchiKey: MNNWRIQCBSTKNP-UHFFFAOYSA-N

Formula: C21H42

SMILES: C=C(C)CCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 294.56

Physical Properties

Property code	Value	Unit	Source
gf	205.23	kJ/mol	Joback Method
hf	-361.13	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	61.75	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	8.214		Crippen Method
mcvol	302.450	ml/mol	McGowan Method
pc	984.55	kPa	Joback Method
rinpol	2091.00		NIST Webbook
tb	676.44	K	Joback Method
tc	840.60	K	Joback Method
tf	310.71	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.07	J/mol×K	676.44	Joback Method
cpg	897.10	J/mol×K	703.80	Joback Method
cpg	917.23	J/mol×K	731.16	Joback Method
cpg	936.50	J/mol×K	758.52	Joback Method
cpg	954.93	J/mol×K	785.88	Joback Method
cpg	972.56	J/mol×K	813.24	Joback Method
cpg	989.42	J/mol×K	840.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R205791&Units=SI

Legend

cpg:	Ideal gas heat capacity
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