

9-Heptatricosene

Inchi: InChI=1S/C37H74/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-36-34-32-30-28-26-24-22-20-18-16-14-12-10-8-6-4-2-1
InchiKey: RRHTUONHMBXKV-HTXNQAPBSA-N
Formula: C37H74
SMILES: CCCCCCCC=CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 518.98

Physical Properties

Property code	Value	Unit	Source
gf	340.88	kJ/mol	Joback Method
hf	-689.79	kJ/mol	Joback Method
hfus	91.79	kJ/mol	Joback Method
hvap	97.91	kJ/mol	Joback Method
log10ws	-15.16		Crippen Method
logp	14.456		Crippen Method
mvol	527.890	ml/mol	McGowan Method
pc	449.25	kPa	Joback Method
rinpol	3686.00		NIST Webbook
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tb	1050.12	K	Joback Method
tc	1348.55	K	Joback Method
tf	501.67	K	Joback Method
vc	2.087	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1937.29	J/molxK	1050.12	Joback Method
cpg	1973.83	J/molxK	1099.86	Joback Method
cpg	2007.89	J/molxK	1149.60	Joback Method
cpg	2039.83	J/molxK	1199.33	Joback Method
cpg	2069.99	J/molxK	1249.07	Joback Method
cpg	2098.73	J/molxK	1298.81	Joback Method
cpg	2126.40	J/molxK	1348.55	Joback Method
dvisc	0.0003623	Paxs	501.67	Joback Method

dvisc	0.0001138	Paxs	593.08	Joback Method
dvisc	0.0000487	Paxs	684.49	Joback Method
dvisc	0.0000254	Paxs	775.89	Joback Method
dvisc	0.0000152	Paxs	867.30	Joback Method
dvisc	0.0000101	Paxs	958.71	Joback Method
dvisc	0.0000071	Paxs	1050.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R608596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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