

3,9,15,21-tetramethylheptatriacontane

Inchi: InChI=1S/C41H84/c1-7-9-10-11-12-13-14-15-16-17-18-19-20-24-32-39(4)34-27-22-28-30
InchiKey: BJFUMFVAERSXGO-UHFFFAOYSA-N
Formula: C41H84
SMILES: CCCCCCCCCCCCCCCCC(C)CCCCC(C)CCCCC(C)CCCCC(C)CC
Mol. weight [g/mol]: 577.11

Physical Properties

Property code	Value	Unit	Source
gf	284.58	kJ/mol	Joback Method
hf	-910.69	kJ/mol	Joback Method
hfus	87.85	kJ/mol	Joback Method
hvap	105.31	kJ/mol	Joback Method
log10ws	-16.02		Crippen Method
logp	15.664		Crippen Method
mcvol	588.550	ml/mol	McGowan Method
pc	381.17	kPa	Joback Method
rinpol	3865.00		NIST Webbook
tb	1135.72	K	Joback Method
tc	1509.28	K	Joback Method
tf	491.83	K	Joback Method
vc	2.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2246.46	J/molxK	1135.72	Joback Method
cpg	2288.95	J/molxK	1197.98	Joback Method
cpg	2327.47	J/molxK	1260.24	Joback Method
cpg	2362.69	J/molxK	1322.50	Joback Method
cpg	2395.30	J/molxK	1384.76	Joback Method
cpg	2426.00	J/molxK	1447.02	Joback Method
cpg	2455.47	J/molxK	1509.28	Joback Method
dvisc	0.0004135	Paxs	491.83	Joback Method
dvisc	0.0000857	Paxs	599.14	Joback Method

dvisc	0.0000286	Paxs	706.46	Joback Method
dvisc	0.0000128	Paxs	813.78	Joback Method
dvisc	0.0000069	Paxs	921.09	Joback Method
dvisc	0.0000042	Paxs	1028.40	Joback Method
dvisc	0.0000028	Paxs	1135.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R280207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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