

dimethyl-2,13 tetradecadiene-1,13

Inchi:	InChI=1S/C16H30/c1-15(2)13-11-9-7-5-6-8-10-12-14-16(3)4/h1,3,5-14H2,2,4H3
InchiKey:	YUBFSDANSPWHJV-UHFFFAOYSA-N
Formula:	C16H30
SMILES:	C=C(C)CCCCCCCCCCC(=C)C
Mol. weight [g/mol]:	222.41

Physical Properties

Property code	Value	Unit	Source
gf	242.42	kJ/mol	Joback Method
hf	-142.29	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	50.03	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	6.040		Crippen Method
mcvol	227.700	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1706.00		NIST Webbook
tb	558.60	K	Joback Method
tc	726.67	K	Joback Method
tf	238.64	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.77	J/molxK	558.60	Joback Method
cpg	588.56	J/molxK	586.61	Joback Method
cpg	606.53	J/molxK	614.62	Joback Method
cpg	623.73	J/molxK	642.63	Joback Method
cpg	640.17	J/molxK	670.65	Joback Method
cpg	655.90	J/molxK	698.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R242507&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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