

6,10,14-Trimethylpentadeca-3,5-diene-2-one

Inchi: InChI=1S/C18H32O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h8,13-16H,6-7,9
InchiKey: LGSXJEDIGQMTRC-BYYJQVKUSA-N
Formula: C18H32O
SMILES: CC(=O)C=CC=C(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 264.45
CAS: 1604-32-6

Physical Properties

Property code	Value	Unit	Source
chl	-11208.90 ± 4.30	kJ/mol	NIST Webbook
chl	-11205.40	kJ/mol	NIST Webbook
gf	118.77	kJ/mol	Joback Method
hf	-313.34	kJ/mol	Joback Method
hfl	-451.00 ± 9.10	kJ/mol	NIST Webbook
hfl	-447.60 ± 1.80	kJ/mol	NIST Webbook
hfus	36.02	kJ/mol	Joback Method
hvap	61.63	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.711		Crippen Method
mcvol	257.450	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
tb	672.43	K	Joback Method
tc	856.23	K	Joback Method
tf	288.43	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.66	J/mol×K	672.43	Joback Method
cpg	734.58	J/mol×K	703.06	Joback Method
cpg	752.56	J/mol×K	733.70	Joback Method
cpg	769.65	J/mol×K	764.33	Joback Method
cpg	785.89	J/mol×K	794.97	Joback Method

cpg	801.34	J/mol×K	825.60	Joback Method
cpg	816.04	J/mol×K	856.23	Joback Method
cpl	555.30	J/mol×K	293.95	NIST Webbook
hvapt	43.40 ± 0.50	kJ/mol	482.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1604326&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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

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