1-Phenyldodec-1-en-3-one

Inchi: InChI=1S/C18H26O/c1-2-3-4-5-6-7-11-14-18(19)16-15-17-12-9-8-10-13-17/h8-10,12-13,
InchiKey: SJZSORNQHUZDIP-FOCLMDBBSA-N
Formula: C18H26O
SMILES: CCCCCCCCCC(=O)C=Cc1ccccc1
Mol. weight [g/mol]: 258.40
CAS: 872268-56-9

Physical Properties

Property code	Value	Unit	Source
gf	164.39	kJ/mol	Joback Method
hf	-173.68	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.410		Crippen Method
mcvol	237.990	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2163.40		NIST Webbook
rinpol	2163.40		NIST Webbook
tb	695.95	K	Joback Method
tc	895.04	K	Joback Method
tf	363.89	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.62	J/mol×K	695.95	Joback Method
cpg	737.61	J/mol×K	861.86	Joback Method
cpg	723.64	J/mol×K	828.68	Joback Method
cpg	708.81	J/mol×K	795.50	Joback Method
cpg	693.07	J/mol×K	762.31	Joback Method
cpg	676.36	J/mol×K	729.13	Joback Method
cpg	750.79	J/mol×K	895.04	Joback Method

dvisc	0.0001071	Pa×s	695.95	Joback Method
dvisc	0.0001419	Pa×s	640.61	Joback Method
dvisc	0.0001981	Pa×s	585.26	Joback Method
dvisc	0.0002965	Pa×s	529.92	Joback Method
dvisc	0.0004877	Pa×s	474.58	Joback Method
dvisc	0.0009147	Pa×s	419.23	Joback Method
dvisc	0.0020775	Pa×s	363.89	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=C872268569&Units=SI

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