

Octadecanophenone

Other names:	1-Octadecanone, 1-phenyl- Stearophenone 1-phenyloctadecan-1-one
Inchi:	InChI=1S/C24H40O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-24(25)23-20-17-16-18-
InchiKey:	DBLXXVQTWJFJFI-UHFFFAOYSA-N
Formula:	C24H40O
SMILES:	CCCCCCCCCCCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	344.57
CAS:	6786-36-3

Physical Properties

Property code	Value	Unit	Source
gf	134.69	kJ/mol	Joback Method
hf	-414.74	kJ/mol	Joback Method
hfus	53.56	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.131		Crippen Method
mcvol	326.830	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
tb	829.07	K	Joback Method
tc	1021.62	K	Joback Method
tf	436.59	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.45	J/molxK	829.07	Joback Method
cpg	1055.11	J/molxK	861.16	Joback Method
cpg	1073.65	J/molxK	893.25	Joback Method
cpg	1091.13	J/molxK	925.35	Joback Method
cpg	1107.60	J/molxK	957.44	Joback Method
cpg	1123.13	J/molxK	989.53	Joback Method

cpg	1137.78	J/mol×K	1021.62	Joback Method
dvisc	0.0012519	Paxs	436.59	Joback Method
dvisc	0.0005348	Paxs	502.00	Joback Method
dvisc	0.0002779	Paxs	567.42	Joback Method
dvisc	0.0001654	Paxs	632.83	Joback Method
dvisc	0.0001085	Paxs	698.24	Joback Method
dvisc	0.0000765	Paxs	763.66	Joback Method
dvisc	0.0000570	Paxs	829.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6786363&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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