Benzaldehyde, 4-(octyloxy)-

Other names:	4-Octyloxybenzaldehyde
	p-Octyloxybenzaldehyde
	p-n-Octoxy benzaldehyde
	4-n-Octyloxybenzaldehyde
	p-n-Octyloxybenzaldehyde
Inchi:	InChI=1S/C15H22O2/c1-2-3-4-5-6-7-12-17-15-10-8-14(13-16)9-11-15/h8-11,13H,2-7,12H
InchiKey:	KVOWZHASDIKNFK-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCCCCCCCOc1ccc(C=O)cc1
Mol. weight [g/mol]:	234.33
CAS:	24083-13-4

Physical Properties

Property code	Value	Unit	Source
gf	-26.32	kJ/mol	Joback Method
hf	-345.67	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.238		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
tb	645.34	K	Joback Method
tc	839.84	K	Joback Method
tf	361.98	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.04	J/mol×K	645.34	Joback Method
cpg	619.11	J/mol×K	807.43	Joback Method
cpg	606.14	J/mol×K	775.01	Joback Method
cpg	592.37	J/mol×K	742.59	Joback Method

cpg	577.78	J/mol×K	710.17	Joback Method
cpg	562.35	J/mol×K	677.76	Joback Method
cpg	631.30	J/mol×K	839.84	Joback Method
dvisc	0.0001492	Pa×s	645.34	Joback Method
dvisc	0.0001910	Pa×s	598.11	Joback Method
dvisc	0.0002551	Pa×s	550.89	Joback Method
dvisc	0.0003597	Pa×s	503.66	Joback Method
dvisc	0.0005447	Pa×s	456.43	Joback Method
dvisc	0.0009078	Pa×s	409.21	Joback Method
dvisc	0.0017284	Pa×s	361.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.50 ± 0.50	K	0.10	NIST Webbook

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=C24083134&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume