

Methyl 4-octyloxybenzoate

Other names:	Benzoic acid, 4-(octyloxy)-, methyl ester benzoic acid, 4-n-octyloxy-, methyl ester
Inchi:	InChI=1S/C16H24O3/c1-3-4-5-6-7-8-13-19-15-11-9-14(10-12-15)16(17)18-2/h9-12H,3-8,
InchiKey:	JCVLYBQFVTYGKT-UHFFFAOYSA-N
Formula:	C16H24O3
SMILES:	CCCCCCCCOc1ccc(C(=O)OC)cc1
Mol. weight [g/mol]:	264.36
CAS:	62435-37-4

Physical Properties

Property code	Value	Unit	Source
gf	-152.30	kJ/mol	Joback Method
hf	-525.53	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.213		Crippen Method
mvol	225.850	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
tb	695.85	K	Joback Method
tc	890.88	K	Joback Method
tf	403.41	K	Joback Method
vc	0.866	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.30	J/mol×K	695.85	Joback Method
cpg	644.95	J/mol×K	728.35	Joback Method
cpg	660.67	J/mol×K	760.86	Joback Method
cpg	675.49	J/mol×K	793.36	Joback Method
cpg	689.41	J/mol×K	825.87	Joback Method
cpg	702.45	J/mol×K	858.37	Joback Method
cpg	714.61	J/mol×K	890.88	Joback Method

dvisc	0.0010218	Paxs	403.41	Joback Method
dvisc	0.0005542	Paxs	452.15	Joback Method
dvisc	0.0003386	Paxs	500.89	Joback Method
dvisc	0.0002257	Paxs	549.63	Joback Method
dvisc	0.0001608	Paxs	598.37	Joback Method
dvisc	0.0001205	Paxs	647.11	Joback Method
dvisc	0.0000941	Paxs	695.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62435374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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