Benzeneacetic acid, octyl ester

Other names: octyl phenylacetate
Inchi: InChI=1S/C16H24O2/c1-2-3-4-5-6-10-13-18-16(17)14-15-11-8-7-9-12-15/h7-9,11-12H,2-
InchiKey: VGYPAVUJUMQTGE-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CCCCCCCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]: 248.36
CAS: 122-45-2

Physical Properties

Property code	Value	Unit	Source
gf	-37.67	kJ/mol	Joback Method
hf	-381.84	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.133		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1830.31		NIST Webbook
rinpol	1800.30		NIST Webbook
rinpol	1800.30		NIST Webbook
tb	668.45	K	Joback Method
tc	863.72	K	Joback Method
tf	368.66	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.99	J/mol×K	668.45	Joback Method
cpg	617.16	J/mol×K	701.00	Joback Method
cpg	633.37	J/mol×K	733.54	Joback Method
cpg	648.65	J/mol×K	766.09	Joback Method
cpg	663.03	J/mol×K	798.63	Joback Method

cpg	676.54	J/mol×K	831.18	Joback Method
cpg	689.21	J/mol×K	863.72	Joback Method
dvisc	0.0018111	Pa×s	368.66	Joback Method
dvisc	0.0008831	Pa×s	418.62	Joback Method
dvisc	0.0005018	Pa×s	468.59	Joback Method
dvisc	0.0003180	Pa×s	518.55	Joback Method
dvisc	0.0002183	Pa×s	568.52	Joback Method
dvisc	0.0001593	Pa×s	618.48	Joback Method
dvisc	0.0001218	Pa×s	668.45	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=C122452&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