octyl hydrogen phthalate

Other names: 2-(Octyloxycarbonyl)benzoic acid
Inchi: InChI=1S/C16H22O4/c1-2-3-4-5-6-9-12-20-16(19)14-11-8-7-10-13(14)15(17)18/h7-8,10-
InchiKey: PKIYFBICNICNGJ-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 278.34
CAS: 5393-19-1

Physical Properties

Property code	Value	Unit	Source
gf	-313.04	kJ/mol	Joback Method
hf	-658.12	kJ/mol	Joback Method
hfus	39.32	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.902		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	819.48	K	Joback Method
tc	1017.75	K	Joback Method
tf	491.93	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.76	J/mol×K	819.48	Joback Method
cpg	691.54	J/mol×K	852.53	Joback Method
cpg	703.46	J/mol×K	885.57	Joback Method
cpg	714.54	J/mol×K	918.62	Joback Method
cpg	724.81	J/mol×K	951.66	Joback Method
cpg	734.30	J/mol×K	984.71	Joback Method

cpg	743.02	J/mol×K	1017.75	Joback Method
dvisc	0.0006051	Pa×s	491.93	Joback Method
dvisc	0.0002614	Pa×s	546.52	Joback Method
dvisc	0.0001315	Pa×s	601.11	Joback Method
dvisc	0.0000742	Pa×s	655.70	Joback Method
dvisc	0.0000457	Pa×s	710.30	Joback Method
dvisc	0.0000302	Pa×s	764.89	Joback Method
dvisc	0.0000211	Pa×s	819.48	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5393191&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

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

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