hexyl hydrogen phthalate

Other names: 2-(Hexyloxycarbonyl)benzoic acid
Inchi: InChI=1S/C14H18O4/c1-2-3-4-7-10-18-14(17)12-9-6-5-8-11(12)13(15)16/h5-6,8-9H,2-4,7
InchiKey: XOSNGXNHDRYFEF-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 250.29
CAS: 24539-57-9

Physical Properties

Property code	Value	Unit	Source
gf	-329.88	kJ/mol	Joback Method
hf	-616.84	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	82.28	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.122		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	773.72	K	Joback Method
tc	972.49	K	Joback Method
tf	469.39	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.52	J/mol×K	773.72	Joback Method
cpg	620.70	J/mol×K	939.36	Joback Method
cpg	611.76	J/mol×K	906.23	Joback Method
cpg	602.09	J/mol×K	873.11	Joback Method
cpg	591.67	J/mol×K	839.98	Joback Method
cpg	580.49	J/mol×K	806.85	Joback Method

cpg	628.93	J/mol×K	972.49	Joback Method
dvisc	0.0000298	Pa×s	773.72	Joback Method
dvisc	0.0000426	Pa×s	723.00	Joback Method
dvisc	0.0000643	Pa×s	672.28	Joback Method
dvisc	0.0001037	Pa×s	621.55	Joback Method
dvisc	0.0001823	Pa×s	570.83	Joback Method
dvisc	0.0003578	Pa×s	520.11	Joback Method
dvisc	0.0008120	Pa×s	469.39	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=C24539579&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

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