decyl hydrogen phthalate

Other names: 2-(Decyloxycarbonyl)benzoic acid
Inchi: InChI=1S/C18H26O4/c1-2-3-4-5-6-7-8-11-14-22-18(21)16-13-10-9-12-15(16)17(19)20/h9
InchiKey: FEFCILUKYGHITK-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 306.40
CAS: 24539-60-4

Physical Properties

Property code	Value	Unit	Source
gf	-296.20	kJ/mol	Joback Method
hf	-699.40	kJ/mol	Joback Method
hfus	44.50	kJ/mol	Joback Method
hvap	91.18	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.682		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	865.24	K	Joback Method
tc	1065.69	K	Joback Method
tf	514.47	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.77	J/mol×K	865.24	Joback Method
cpg	851.18	J/mol×K	1032.28	Joback Method
cpg	841.26	J/mol×K	998.87	Joback Method
cpg	830.49	J/mol×K	965.46	Joback Method
cpg	818.84	J/mol×K	932.06	Joback Method
cpg	806.28	J/mol×K	898.65	Joback Method

cpg	860.28	J/mol×K	1065.69	Joback Method
dvisc	0.0000148	Pa×s	865.24	Joback Method
dvisc	0.0000213	Pa×s	806.78	Joback Method
dvisc	0.0000323	Pa×s	748.32	Joback Method
dvisc	0.0000528	Pa×s	689.86	Joback Method
dvisc	0.0000942	Pa×s	631.39	Joback Method
dvisc	0.0001895	Pa×s	572.93	Joback Method
dvisc	0.0004465	Pa×s	514.47	Joback Method

Sources

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=C24539604&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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