Phthalic acid, decyl methyl ester

Other names: ,2-Benzenedicarboxylic acid, decyl methyl ester
Inchi: InChI=1S/C19H28O4/c1-3-4-5-6-7-8-9-12-15-23-19(21)17-14-11-10-13-16(17)18(20)22-2
InchiKey: OXRWHMFJAPZSRT-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
af	0.9687		Cheméo Relay (1.0)
hf	-786.93	kJ/mol	Cheméo Relay (1.0)
hfus	44.19	kJ/mol	Joback Method
hvap	98.67	kJ/mol	Cheméo Relay (1.0)
ie	9.22	eV	Cheméo Relay (1.0)
log10ws	-5.72		Cheméo Relay (1.0)
logp	4.771		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2346.00		NIST Webbook
tb	620.67	K	Cheméo Relay (1.0)
tc	828.59	K	Cheméo Relay (1.0)
tf	277.13	K	Cheméo Relay (1.0)
vc	1.018	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.06	J/mol×K	818.36	Joback Method
cpg	834.97	J/mol×K	851.61	Joback Method
cpg	849.80	J/mol×K	884.86	Joback Method
cpg	863.56	J/mol×K	918.12	Joback Method
cpg	876.27	J/mol×K	951.37	Joback Method
cpg	887.96	J/mol×K	984.62	Joback Method
cpg	898.65	J/mol×K	1017.87	Joback Method

dvisc	0.0006541	Pa×s	487.15	Joback Method
dvisc	0.0003630	Pa×s	542.35	Joback Method
dvisc	0.0002246	Pa×s	597.55	Joback Method
dvisc	0.0001507	Pa×s	652.75	Joback Method
dvisc	0.0001077	Pa×s	707.96	Joback Method
dvisc	0.0000807	Pa×s	763.16	Joback Method
dvisc	0.0000629	Pa×s	818.36	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C256481386&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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