Phthalic acid, decyl 2-methoxybenzyl ester

Inchi: InChI=1S/C26H34O5/c1-3-4-5-6-7-8-9-14-19-30-25(27)22-16-11-12-17-23(22)26(28)31-2
InchiKey: WXVRKHLBKSMDQK-UHFFFAOYSA-N
Formula: C26H34O5
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1OC
Mol. weight [g/mol]: 426.55

Physical Properties

Property code	Value	Unit	Source
gf	-199.24	kJ/mol	Joback Method
hf	-751.67	kJ/mol	Joback Method
hfus	57.16	kJ/mol	Joback Method
hvap	100.07	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	6.350		Crippen Method
mcvol	350.430	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	3573.00		NIST Webbook
rinpol	3573.00		NIST Webbook
tb	1032.60	K	Joback Method
tc	1264.59	K	Joback Method
tf	627.21	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.68	J/mol×K	1032.60	Joback Method
cpg	1213.47	J/mol×K	1225.93	Joback Method
cpg	1206.78	J/mol×K	1187.26	Joback Method
cpg	1198.49	J/mol×K	1148.60	Joback Method
cpg	1188.57	J/mol×K	1109.93	Joback Method
cpg	1176.98	J/mol×K	1071.27	Joback Method
cpg	1218.62	J/mol×K	1264.59	Joback Method
dvisc	0.0000179	Pa×s	1032.60	Joback Method

dvisc	0.0000228	Pa×s	965.03	Joback Method
dvisc	0.0000301	Pa×s	897.47	Joback Method
dvisc	0.0000417	Pa×s	829.90	Joback Method
dvisc	0.0000612	Pa×s	762.34	Joback Method
dvisc	0.0000966	Pa×s	694.77	Joback Method
dvisc	0.0001683	Pa×s	627.21	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=U382499&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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