

Phthalic acid, 2-methylbenzyl undecyl ester

Inchi: InChI=1S/C27H36O4/c1-3-4-5-6-7-8-9-10-15-20-30-26(28)24-18-13-14-19-25(24)27(29)3
InchiKey: HFKRYQCBGYDZNH-UHFFFAOYSA-N
Formula: C27H36O4
SMILES: CCCCCCCCCCOC(=O)c1cccc1C(=O)OCc1cccc1C
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-85.82	kJ/mol	Joback Method
hf	-640.09	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	99.88	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	7.040		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1050.05	kPa	Joback Method
rinpol	3061.00		NIST Webbook
tb	1033.06	K	Joback Method
tc	1265.06	K	Joback Method
tf	616.25	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.89	J/molxK	1033.06	Joback Method
cpg	1212.40	J/molxK	1071.73	Joback Method
cpg	1225.34	J/molxK	1110.39	Joback Method
cpg	1236.78	J/molxK	1149.06	Joback Method
cpg	1246.78	J/molxK	1187.73	Joback Method
cpg	1255.41	J/molxK	1226.39	Joback Method
cpg	1262.73	J/molxK	1265.06	Joback Method
dvisc	0.0002136	Paxs	616.25	Joback Method
dvisc	0.0001191	Paxs	685.72	Joback Method

dvisc	0.0000739	Paxs	755.19	Joback Method
dvisc	0.0000497	Paxs	824.65	Joback Method
dvisc	0.0000356	Paxs	894.12	Joback Method
dvisc	0.0000267	Paxs	963.59	Joback Method
dvisc	0.0000209	Paxs	1033.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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