

Phthalic acid, 3-methoxybenzyl nonyl ester

Inchi: InChI=1S/C25H32O5/c1-3-4-5-6-7-8-11-17-29-24(26)22-15-9-10-16-23(22)25(27)30-19-2
InchiKey: RNVCMTMTALCQIP-UHFFFAOYSA-N
Formula: C25H32O5
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]: 412.52

Physical Properties

Property code	Value	Unit	Source
gf	-207.66	kJ/mol	Joback Method
hf	-731.03	kJ/mol	Joback Method
hfus	54.57	kJ/mol	Joback Method
hvap	97.84	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.960		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	3099.00		NIST Webbook
tb	1009.72	K	Joback Method
tc	1238.04	K	Joback Method
tf	615.94	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.18	J/molxK	1009.72	Joback Method
cpg	1116.51	J/molxK	1047.77	Joback Method
cpg	1128.20	J/molxK	1085.83	Joback Method
cpg	1138.30	J/molxK	1123.88	Joback Method
cpg	1146.83	J/molxK	1161.93	Joback Method
cpg	1153.84	J/molxK	1199.98	Joback Method
cpg	1159.35	J/molxK	1238.04	Joback Method
dvisc	0.0001892	Paxs	615.94	Joback Method
dvisc	0.0001097	Paxs	681.57	Joback Method

dvisc	0.0000700	Paxs	747.20	Joback Method
dvisc	0.0000480	Paxs	812.83	Joback Method
dvisc	0.0000348	Paxs	878.46	Joback Method
dvisc	0.0000264	Paxs	944.09	Joback Method
dvisc	0.0000208	Paxs	1009.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377982&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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