

Phthalic acid, dodecyl 2-methoxybenzyl ester

Inchi:	InChI=1S/C28H38O5/c1-3-4-5-6-7-8-9-10-11-16-21-32-27(29)24-18-13-14-19-25(24)28(30)26
InchiKey:	HHGMBHZPKWZHIU-UHFFFAOYSA-N
Formula:	C28H38O5
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1OC
Mol. weight [g/mol]:	454.60

Physical Properties

Property code	Value	Unit	Source
gf	-182.40	kJ/mol	Joback Method
hf	-792.95	kJ/mol	Joback Method
hfus	62.34	kJ/mol	Joback Method
hvap	104.52	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.130		Crippen Method
mvol	378.610	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	3774.00		NIST Webbook
rinpol	3774.00		NIST Webbook
tb	1078.36	K	Joback Method
tc	1320.98	K	Joback Method
tf	649.75	K	Joback Method
vc	1.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.63	J/molxK	1078.36	Joback Method
cpg	1298.89	J/molxK	1118.80	Joback Method
cpg	1310.23	J/molxK	1159.23	Joback Method
cpg	1319.72	J/molxK	1199.67	Joback Method
cpg	1327.41	J/molxK	1240.10	Joback Method
cpg	1333.35	J/molxK	1280.54	Joback Method
cpg	1337.60	J/molxK	1320.98	Joback Method
dvisc	0.0001320	Paxs	649.75	Joback Method

dvisc	0.0000743	Paxs	721.19	Joback Method
dvisc	0.0000464	Paxs	792.62	Joback Method
dvisc	0.0000313	Paxs	864.06	Joback Method
dvisc	0.0000224	Paxs	935.49	Joback Method
dvisc	0.0000169	Paxs	1006.93	Joback Method
dvisc	0.0000132	Paxs	1078.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382501&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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