

Isophthalic acid, decyl 3-phenylpropyl ester

Inchi: InChI=1S/C27H36O4/c1-2-3-4-5-6-7-8-12-20-30-26(28)24-18-13-19-25(22-24)27(29)31-2
InchiKey: JCAYKSCPHVYNKP-UHFFFAOYSA-N
Formula: C27H36O4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-76.19	kJ/mol	Joback Method
hf	-628.62	kJ/mol	Joback Method
hfus	58.95	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	6.774		Crippen Method
mvol	358.650	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	3427.00		NIST Webbook
rinpol	3427.00		NIST Webbook
tb	1028.08	K	Joback Method
tc	1259.02	K	Joback Method
tf	603.73	K	Joback Method
vc	1.379	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.95	J/molxK	1028.08	Joback Method
cpg	1213.64	J/molxK	1066.57	Joback Method
cpg	1226.81	J/molxK	1105.06	Joback Method
cpg	1238.53	J/molxK	1143.55	Joback Method
cpg	1248.86	J/molxK	1182.04	Joback Method
cpg	1257.89	J/molxK	1220.53	Joback Method
cpg	1265.69	J/molxK	1259.02	Joback Method
dvisc	0.0002386	Paxs	603.73	Joback Method

dvisc	0.0001276	Paxs	674.46	Joback Method
dvisc	0.0000768	Paxs	745.18	Joback Method
dvisc	0.0000505	Paxs	815.90	Joback Method
dvisc	0.0000355	Paxs	886.63	Joback Method
dvisc	0.0000263	Paxs	957.35	Joback Method
dvisc	0.0000203	Paxs	1028.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344392&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

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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