

Isophthalic acid, dodecyl hept-2-yl ester

Inchi:	InChI=1S/C27H44O4/c1-4-6-8-9-10-11-12-13-14-16-21-30-26(28)24-19-17-20-25(22-24)
InchiKey:	AFWBWVGEQHRFCD-UHFFFAOYSA-N
Formula:	C27H44O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCC)c1
Mol. weight [g/mol]:	432.64

Physical Properties

Property code	Value	Unit	Source
gf	-191.04	kJ/mol	Joback Method
hf	-870.43	kJ/mol	Joback Method
hfus	61.39	kJ/mol	Joback Method
hvap	96.56	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	7.890		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	868.11	kPa	Joback Method
rinsol	3037.00		NIST Webbook
tb	1000.96	K	Joback Method
tc	1226.87	K	Joback Method
tf	562.31	K	Joback Method
vc	1.482	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.77	J/molxK	1000.96	Joback Method
cpg	1379.63	J/molxK	1189.22	Joback Method
cpg	1368.14	J/molxK	1151.57	Joback Method
cpg	1355.17	J/molxK	1113.92	Joback Method
cpg	1340.65	J/molxK	1076.26	Joback Method
cpg	1324.54	J/molxK	1038.61	Joback Method
cpg	1389.70	J/molxK	1226.87	Joback Method
dvisc	0.0000178	Paxs	1000.96	Joback Method
dvisc	0.0000236	Paxs	927.85	Joback Method

dvisc	0.0000330	Paxs	854.74	Joback Method
dvisc	0.0000489	Paxs	781.63	Joback Method
dvisc	0.0000788	Paxs	708.53	Joback Method
dvisc	0.0001415	Paxs	635.42	Joback Method
dvisc	0.0002962	Paxs	562.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356534&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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