

Isophthalic acid, hexyl tridec-2-ynyl ester

Inchi: InChI=1S/C27H40O4/c1-3-5-7-9-10-11-12-13-14-15-17-22-31-27(29)25-20-18-19-24(23-
InchiKey: INSAPBRYHXRYBL-UHFFFAOYSA-N
Formula: C27H40O4
SMILES: CCCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCCCCC)c1
Mol. weight [g/mol]: 428.60

Physical Properties

Property code	Value	Unit	Source
gf	14.20	kJ/mol	Joback Method
hf	-592.85	kJ/mol	Joback Method
hfus	68.03	kJ/mol	Joback Method
hvap	99.10	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.115		Crippen Method
mvol	373.810	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	3282.00		NIST Webbook
rinpol	3282.00		NIST Webbook
tb	1010.40	K	Joback Method
tc	1237.04	K	Joback Method
tf	683.41	K	Joback Method
vc	1.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.45	J/molxK	1010.40	Joback Method
cpg	1265.92	J/molxK	1048.17	Joback Method
cpg	1280.82	J/molxK	1085.95	Joback Method
cpg	1294.22	J/molxK	1123.72	Joback Method
cpg	1306.15	J/molxK	1161.49	Joback Method
cpg	1316.68	J/molxK	1199.27	Joback Method
cpg	1325.85	J/molxK	1237.04	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=U343918&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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