

Isophthalic acid, ethyl tridec-2-ynyl ester

Inchi:	InChI=1S/C23H32O4/c1-3-5-6-7-8-9-10-11-12-13-14-18-27-23(25)21-17-15-16-20(19-21
InchiKey:	YIVXZOWRVNKJIO-UHFFFAOYSA-N
Formula:	C23H32O4
SMILES:	CCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCC)c1
Mol. weight [g/mol]:	372.50

Physical Properties

Property code	Value	Unit	Source
gf	-19.48	kJ/mol	Joback Method
hf	-510.29	kJ/mol	Joback Method
hfus	57.67	kJ/mol	Joback Method
hvap	90.19	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	5.554		Crippen Method
mvol	317.450	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tb	918.88	K	Joback Method
tc	1132.03	K	Joback Method
tf	638.33	K	Joback Method
vc	1.226	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.00	J/molxK	918.88	Joback Method
cpg	1019.84	J/molxK	954.41	Joback Method
cpg	1034.38	J/molxK	989.93	Joback Method
cpg	1047.66	J/molxK	1025.46	Joback Method
cpg	1059.71	J/molxK	1060.98	Joback Method
cpg	1070.55	J/molxK	1096.51	Joback Method
cpg	1080.23	J/molxK	1132.03	Joback Method

Sources

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=U343912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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