

Isophthalic acid, propyl tridec-2-ynyl ester

Inchi:	InChI=1S/C24H34O4/c1-3-5-6-7-8-9-10-11-12-13-14-19-28-24(26)22-17-15-16-21(20-22
InchiKey:	QJCVBXCOHUVOLQ-UHFFFAOYSA-N
Formula:	C24H34O4
SMILES:	CCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCCC)c1
Mol. weight [g/mol]:	386.52

Physical Properties

Property code	Value	Unit	Source
gf	-11.06	kJ/mol	Joback Method
hf	-530.93	kJ/mol	Joback Method
hfus	60.26	kJ/mol	Joback Method
hvap	92.42	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	5.944		Crippen Method
mvol	331.540	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	2976.00		NIST Webbook
rinpol	2976.00		NIST Webbook
tb	941.76	K	Joback Method
tc	1156.88	K	Joback Method
tf	649.60	K	Joback Method
vc	1.282	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.60	J/mol×K	941.76	Joback Method
cpg	1080.57	J/mol×K	977.61	Joback Method
cpg	1095.20	J/mol×K	1013.47	Joback Method
cpg	1108.51	J/mol×K	1049.32	Joback Method
cpg	1120.55	J/mol×K	1085.17	Joback Method
cpg	1131.35	J/mol×K	1121.03	Joback Method
cpg	1140.93	J/mol×K	1156.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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