

Isophthalic acid, heptyl tridec-2-ynyl ester

Inchi:	InChI=1S/C28H42O4/c1-3-5-7-9-10-11-12-13-14-16-18-23-32-28(30)26-21-19-20-25(24-
InchiKey:	QCYWCKVYXUYRJM-UHFFFAOYSA-N
Formula:	C28H42O4
SMILES:	CCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCCCCCCC)c1
Mol. weight [g/mol]:	442.63

Physical Properties

Property code	Value	Unit	Source
gf	22.62	kJ/mol	Joback Method
hf	-613.49	kJ/mol	Joback Method
hfus	70.62	kJ/mol	Joback Method
hvap	101.32	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	7.505		Crippen Method
mvol	387.900	ml/mol	McGowan Method
pc	897.49	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1033.28	K	Joback Method
tc	1265.85	K	Joback Method
tf	694.68	K	Joback Method
vc	1.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.92	J/mol×K	1033.28	Joback Method
cpg	1328.59	J/mol×K	1072.04	Joback Method
cpg	1343.61	J/mol×K	1110.80	Joback Method
cpg	1357.02	J/mol×K	1149.57	Joback Method
cpg	1368.90	J/mol×K	1188.33	Joback Method
cpg	1379.30	J/mol×K	1227.09	Joback Method
cpg	1388.28	J/mol×K	1265.85	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=U343919&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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