

Isophthalic acid, butyl hex-4-yn-3-yl ester

Inchi:	InChI=1S/C18H22O4/c1-4-7-12-21-17(19)14-10-8-11-15(13-14)18(20)22-16(6-3)9-5-2/h
InchiKey:	MLNWKYQMZHIIHQ-UHFFFAOYSA-N
Formula:	C18H22O4
SMILES:	CC#CC(CC)OC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]:	302.36

Physical Properties

Property code	Value	Unit	Source
gf	-64.02	kJ/mol	Joback Method
hf	-412.37	kJ/mol	Joback Method
hfus	41.20	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.602		Crippen Method
mvol	247.000	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
tb	804.04	K	Joback Method
tc	1021.90	K	Joback Method
tf	566.98	K	Joback Method
vc	0.940	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.88	J/molxK	804.04	Joback Method
cpg	727.14	J/molxK	840.35	Joback Method
cpg	741.25	J/molxK	876.66	Joback Method
cpg	754.24	J/molxK	912.97	Joback Method
cpg	766.11	J/molxK	949.28	Joback Method
cpg	776.88	J/molxK	985.59	Joback Method
cpg	786.57	J/molxK	1021.90	Joback Method

Sources

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=U343840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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