Isophthalic acid, butyl 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C23H30O4/c1-6-8-15-26-22(24)19-11-9-12-20(16-19)23(25)27-21(14-13-17(3)

InchiKey: GRBFCFIPCYCOPK-UHFFFAOYSA-N

Formula: C23H30O4

SMILES: C=C(C)C#CC(OC(=O)c1cccc(C(=O)OCCCC)c1)C(C)CCC

Mol. weight [g/mol]: 370.48

Physical Properties

Property code	Value	Unit	Source
gf	54.93	kJ/mol	Joback Method
hf	-405.21	kJ/mol	Joback Method
hfus	48.04	kJ/mol	Joback Method
hvap	88.83	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.185		Crippen Method
mcvol	313.150	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
tb	914.56	K	Joback Method
tc	1133.78	K	Joback Method
tf	592.61	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.88	J/mol×K	914.56	Joback Method
cpg	991.59	J/mol×K	951.10	Joback Method
cpg	1005.98	J/mol×K	987.63	Joback Method
cpg	1019.10	J/mol×K	1024.17	Joback Method
cpg	1030.98	J/mol×K	1060.71	Joback Method
cpg	1041.66	J/mol×K	1097.24	Joback Method
cpg	1051.17	J/mol×K	1133.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U343855&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume