

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

Inchi: InChI=1S/C21H26O4/c1-6-9-16(5)19(13-12-15(3)4)25-21(23)18-11-8-10-17(14-18)20(22)
InchiKey: BZDFPOMORSPWJX-UHFFFAOYSA-N
Formula: C21H26O4
SMILES: C=C(C)C#CC(OC(=O)c1cccc(C(=O)OCC)c1)C(C)CCC
Mol. weight [g/mol]: 342.43

Physical Properties

Property code	Value	Unit	Source
gf	38.09	kJ/mol	Joback Method
hf	-363.93	kJ/mol	Joback Method
hfus	42.86	kJ/mol	Joback Method
hvap	84.38	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.404		Crippen Method
mvol	284.970	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2397.00		NIST Webbook
rinpol	2397.00		NIST Webbook
tb	868.80	K	Joback Method
tc	1089.27	K	Joback Method
tf	570.07	K	Joback Method
vc	1.083	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.54	J/mol×K	868.80	Joback Method
cpg	873.10	J/mol×K	905.55	Joback Method
cpg	887.40	J/mol×K	942.29	Joback Method
cpg	900.47	J/mol×K	979.04	Joback Method
cpg	912.34	J/mol×K	1015.78	Joback Method
cpg	923.04	J/mol×K	1052.53	Joback Method
cpg	932.62	J/mol×K	1089.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U343853&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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