Isophthalic acid, butyl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C21H28O4/c1-5-7-12-19(14-16(3)4)25-21(23)18-11-9-10-17(15-18)20(22)24-1
InchiKey: ZIVYAAJIMXNBNS-UHFFFAOYSA-N
Formula: C21H28O4
SMILES: CCC#CC(CC(C)C)OC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]: 344.44

Physical Properties

Property code	Value	Unit	Source
gf	-41.20	kJ/mol	Joback Method
hf	-479.57	kJ/mol	Joback Method
hfus	45.45	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.628		Crippen Method
mcvol	289.270	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	872.24	K	Joback Method
tc	1088.29	K	Joback Method
tf	585.79	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.70	J/mol×K	872.24	Joback Method
cpg	901.54	J/mol×K	908.25	Joback Method
cpg	916.09	J/mol×K	944.26	Joback Method
cpg	929.40	J/mol×K	980.26	Joback Method
cpg	941.47	J/mol×K	1016.27	Joback Method
cpg	952.34	J/mol×K	1052.28	Joback Method
cpg	962.03	J/mol×K	1088.29	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=U343925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume