Isophthalic acid, pentyl tridec-2-ynyl ester

Inchi: InChI=1S/C26H38O4/c1-3-5-7-8-9-10-11-12-13-14-16-21-30-26(28)24-19-17-18-23(22-2
InchiKey: QZPNOOOSVJECST-UHFFFAOYSA-N
Formula: C26H38O4
SMILES: CCCCCCCCCCC#CCOC(=O)c1cccc(C(=O)OCCCCC)c1
Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	5.78	kJ/mol	Joback Method
hf	-572.21	kJ/mol	Joback Method
hfus	65.44	kJ/mol	Joback Method
hvap	96.87	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	6.725		Crippen Method
mcvol	359.720	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinpol	3181.00		NIST Webbook
rinpol	3181.00		NIST Webbook
tb	987.52	K	Joback Method
tc	1209.32	K	Joback Method
tf	672.14	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.38	J/mol×K	987.52	Joback Method
cpg	1203.66	J/mol×K	1024.49	Joback Method
cpg	1218.47	J/mol×K	1061.45	Joback Method
cpg	1231.84	J/mol×K	1098.42	Joback Method
cpg	1243.81	J/mol×K	1135.39	Joback Method
cpg	1254.45	J/mol×K	1172.35	Joback Method
cpg	1263.78	J/mol×K	1209.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343916&Units=SI
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

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