Isophthalic acid, di(2-methyloct-5-yn-4-yl) ester

Inchi: InChI=1S/C26H34O4/c1-7-9-14-23(16-19(3)4)29-25(27)21-12-11-13-22(18-21)26(28)30-

InchiKey: XIRGDMCTUKOLGX-UHFFFAOYSA-N

Formula: C26H34O4

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

Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	198.82	kJ/mol	Joback Method
hf	-321.03	kJ/mol	Joback Method
hfus	54.47	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	5.656		Crippen Method
mcvol	351.120	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	2781.00		NIST Webbook
tb	994.76	K	Joback Method
tc	1226.93	K	Joback Method
tf	718.24	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.91	J/mol×K	994.76	Joback Method
cpg	1147.21	J/mol×K	1033.46	Joback Method
cpg	1160.92	J/mol×K	1072.15	Joback Method
cpg	1173.09	J/mol×K	1110.85	Joback Method
cpg	1183.77	J/mol×K	1149.54	Joback Method
cpg	1192.98	J/mol×K	1188.24	Joback Method
cpg	1200.79	J/mol×K	1226.93	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=U343931&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

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