Phthalic acid, undecyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C25H40O4/c1-6-7-8-9-10-11-12-13-16-19-28-23(26)21-17-14-15-18-22(21)24(

InchiKey: UJJUSDNENGWUAH-UHFFFAOYSA-N

Formula: C25H40O4

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-205.04	kJ/mol	Joback Method
hf	-837.90	kJ/mol	Joback Method
hfus	48.79	kJ/mol	Joback Method
hvap	90.81	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.966		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
rinpol	2729.00		NIST Webbook
tb	951.97	K	Joback Method
tc	1166.67	K	Joback Method
tf	542.19	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.74	J/mol×K	951.97	Joback Method
cpg	1254.98	J/mol×K	1130.89	Joback Method
cpg	1242.81	J/mol×K	1095.10	Joback Method
cpg	1229.46	J/mol×K	1059.32	Joback Method
cpg	1214.88	J/mol×K	1023.54	Joback Method
cpg	1198.99	J/mol×K	987.75	Joback Method
cpg	1266.05	J/mol×K	1166.67	Joback Method
dvisc	0.0000185	Pa×s	951.97	Joback Method
dvisc	0.0000249	Pa×s	883.67	Joback Method

dvisc	0.0000352	Pa×s	815.38	Joback Method
dvisc	0.0000530	Pa×s	747.08	Joback Method
dvisc	0.0000868	Pa×s	678.78	Joback Method
dvisc	0.0001587	Pa×s	610.49	Joback Method
dvisc	0.0003378	Pa×s	542.19	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=U357010&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
dvisc:	Dynamic viscosity
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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