

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:	CCCCCCCCCOC(=O)c1cccc1C(=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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.74	J/molxK	951.97	Joback Method
cpg	1198.99	J/molxK	987.75	Joback Method
cpg	1214.88	J/molxK	1023.54	Joback Method
cpg	1229.46	J/molxK	1059.32	Joback Method
cpg	1242.81	J/molxK	1095.10	Joback Method
cpg	1254.98	J/molxK	1130.89	Joback Method
cpg	1266.05	J/molxK	1166.67	Joback Method
dvisc	0.0003378	Paxs	542.19	Joback Method
dvisc	0.0001587	Paxs	610.49	Joback Method

dvisc	0.0000868	Paxs	678.78	Joback Method
dvisc	0.0000530	Paxs	747.08	Joback Method
dvisc	0.0000352	Paxs	815.38	Joback Method
dvisc	0.0000249	Paxs	883.67	Joback Method
dvisc	0.0000185	Paxs	951.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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