

Isophthalic acid, 3,3-dimethylbut-2-yl dodecyl ester

Inchi:	InChI=1S/C26H42O4/c1-6-7-8-9-10-11-12-13-14-15-19-29-24(27)22-17-16-18-23(20-22)
InchiKey:	KJOGNTRKUYZRCC-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)(C)C)c1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-196.62	kJ/mol	Joback Method
hf	-858.54	kJ/mol	Joback Method
hfus	51.38	kJ/mol	Joback Method
hvap	93.04	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.356		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	2895.00		NIST Webbook
rinpol	2895.00		NIST Webbook
tb	974.85	K	Joback Method
tc	1193.64	K	Joback Method
tf	553.46	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.96	J/molxK	974.85	Joback Method
cpg	1261.44	J/molxK	1011.31	Joback Method
cpg	1277.49	J/molxK	1047.78	Joback Method
cpg	1292.20	J/molxK	1084.24	Joback Method
cpg	1305.62	J/molxK	1120.71	Joback Method
cpg	1317.83	J/molxK	1157.17	Joback Method
cpg	1328.91	J/molxK	1193.64	Joback Method
dvisc	0.0002960	Paxs	553.46	Joback Method

dvisc	0.0001378	Paxs	623.69	Joback Method
dvisc	0.0000749	Paxs	693.92	Joback Method
dvisc	0.0000456	Paxs	764.15	Joback Method
dvisc	0.0000301	Paxs	834.39	Joback Method
dvisc	0.0000212	Paxs	904.62	Joback Method
dvisc	0.0000158	Paxs	974.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356557&Units=SI

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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