

Isophthalic acid, decyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C24H38O4/c1-5-6-7-8-9-10-11-12-16-27-23(25)21-14-13-15-22(18-21)24(26)2
InchiKey:	RFVNXQDZWRDEJM-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-218.74	kJ/mol	Joback Method
hf	-813.79	kJ/mol	Joback Method
hfus	50.10	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.575		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	2697.00		NIST Webbook
rinpol	2697.00		NIST Webbook
tb	931.88	K	Joback Method
tc	1142.43	K	Joback Method
tf	513.50	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.29	J/molxK	931.88	Joback Method
cpg	1137.32	J/molxK	966.97	Joback Method
cpg	1152.94	J/molxK	1002.06	Joback Method
cpg	1167.20	J/molxK	1037.16	Joback Method
cpg	1180.14	J/molxK	1072.25	Joback Method
cpg	1191.79	J/molxK	1107.34	Joback Method
cpg	1202.19	J/molxK	1142.43	Joback Method
dvisc	0.0004856	Paxs	513.50	Joback Method

dvisc	0.0002219	Paxs	583.23	Joback Method
dvisc	0.0001198	Paxs	652.96	Joback Method
dvisc	0.0000729	Paxs	722.69	Joback Method
dvisc	0.0000484	Paxs	792.42	Joback Method
dvisc	0.0000343	Paxs	862.15	Joback Method
dvisc	0.0000256	Paxs	931.88	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=U356447&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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