

Isophthalic acid, dodecyl 3-methylpentyl ester

Inchi:	InChI=1S/C26H42O4/c1-4-6-7-8-9-10-11-12-13-14-19-29-25(27)23-16-15-17-24(21-23)2
InchiKey:	PCJBRGMOQVSACW-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CC)c1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-199.46	kJ/mol	Joback Method
hf	-849.79	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.357		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	919.39	kPa	Joback Method
rinpol	3041.00		NIST Webbook
tb	978.08	K	Joback Method
tc	1197.65	K	Joback Method
tf	551.04	K	Joback Method
vc	1.425	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.04	J/molxK	978.08	Joback Method
cpg	1261.53	J/molxK	1014.67	Joback Method
cpg	1277.47	J/molxK	1051.27	Joback Method
cpg	1291.91	J/molxK	1087.86	Joback Method
cpg	1304.90	J/molxK	1124.46	Joback Method
cpg	1316.49	J/molxK	1161.05	Joback Method
cpg	1326.73	J/molxK	1197.65	Joback Method
dvisc	0.0003362	Paxs	551.04	Joback Method
dvisc	0.0001620	Paxs	622.21	Joback Method

dvisc	0.0000907	Paxs	693.39	Joback Method
dvisc	0.0000566	Paxs	764.56	Joback Method
dvisc	0.0000383	Paxs	835.73	Joback Method
dvisc	0.0000275	Paxs	906.91	Joback Method
dvisc	0.0000207	Paxs	978.08	Joback Method

Sources

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=U356549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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