

Isophthalic acid, cis-hex-3-enyl decyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C24H36O4/c1-3-5-7-9-10-11-12-14-19-28-24(26)22-17-15-16-21(20-22)23(25)

IUYZOSIYVUGSCK-VURMDHGXSA-N

C24H36O4

CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCC)c1

388.54

Physical Properties

Property code	Value	Unit	Source
gf	-133.64	kJ/mol	Joback Method
hf	-686.01	kJ/mol	Joback Method
hfus	57.34	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.497		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2847.00		NIST Webbook
tb	936.92	K	Joback Method
tc	1148.38	K	Joback Method
tf	538.42	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.52	J/mol×K	936.92	Joback Method
cpg	1108.15	J/mol×K	972.16	Joback Method
cpg	1123.53	J/mol×K	1007.41	Joback Method
cpg	1137.72	J/mol×K	1042.65	Joback Method
cpg	1150.76	J/mol×K	1077.89	Joback Method
cpg	1162.71	J/mol×K	1113.14	Joback Method
cpg	1173.61	J/mol×K	1148.38	Joback Method
dvisc	0.0003558	Pa×s	538.42	Joback Method
dvisc	0.0001828	Pa×s	604.84	Joback Method

dvisc	0.0001072	Pa×s	671.25	Joback Method
dvisc	0.0000692	Pa×s	737.67	Joback Method
dvisc	0.0000480	Pa×s	804.09	Joback Method
dvisc	0.0000352	Pa×s	870.50	Joback Method
dvisc	0.0000270	Pa×s	936.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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