Isophthalic acid, cis-tetradec-3-enyl isohexyl ester

Inchi: InChI=1S/C28H44O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-21-31-27(29)25-19-16-20-26(23

InchiKey: OJOZKYZRYFPQDL-YPKPFQOOSA-N

Formula: C28H44O4

SMILES: CCCCCCCCCCC=CCCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-102.40	kJ/mol	Joback Method
hf	-773.85	kJ/mol	Joback Method
hfus	64.18	kJ/mol	Joback Method
hvap	98.74	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	7.913		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	846.03	kPa	Joback Method
rinpol	3216.00		NIST Webbook
tb	1028.00	K	Joback Method
tc	1260.74	K	Joback Method
tf	568.50	K	Joback Method
vc	1.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.20	J/mol×K	1028.00	Joback Method
cpg	1415.74	J/mol×K	1221.95	Joback Method
cpg	1403.61	J/mol×K	1183.16	Joback Method
cpg	1390.17	J/mol×K	1144.37	Joback Method
cpg	1375.35	J/mol×K	1105.58	Joback Method
cpg	1359.06	J/mol×K	1066.79	Joback Method
cpg	1426.66	J/mol×K	1260.74	Joback Method
dvisc	0.0000134	Pa×s	1028.00	Joback Method
dvisc	0.0000179	Pa×s	951.42	Joback Method

dvisc	0.0000251	Pa×s	874.83	Joback Method
dvisc	0.0000375	Pa×s	798.25	Joback Method
dvisc	0.0000612	Pa×s	721.67	Joback Method
dvisc	0.0001121	Pa×s	645.08	Joback Method
dvisc	0.0002416	Pa×s	568.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356732&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