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

Inchi: InChI=1S/C26H40O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-29-25(27)23-17-16-18-24(20

InchiKey: BONDHZVIPJVELM-YPKPFQOOSA-N

Formula: C26H40O4

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

Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-119.24	kJ/mol	Joback Method
hf	-732.57	kJ/mol	Joback Method
hfus	59.00	kJ/mol	Joback Method
hvap	94.29	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.133		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	982.24	K	Joback Method
tc	1202.54	K	Joback Method
tf	545.96	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.64	J/mol×K	982.24	Joback Method
cpg	1232.81	J/mol×K	1018.96	Joback Method
cpg	1248.59	J/mol×K	1055.67	Joback Method
cpg	1263.05	J/mol×K	1092.39	Joback Method
cpg	1276.25	J/mol×K	1129.10	Joback Method
cpg	1288.24	J/mol×K	1165.82	Joback Method
cpg	1299.11	J/mol×K	1202.54	Joback Method
dvisc	0.0003119	Pa×s	545.96	Joback Method

dvisc	0.0001471	Pa×s	618.67	Joback Method
dvisc	0.0000812	Pa×s	691.39	Joback Method
dvisc	0.0000502	Pa×s	764.10	Joback Method
dvisc	0.0000338	Pa×s	836.81	Joback Method
dvisc	0.0000242	Pa×s	909.53	Joback Method
dvisc	0.0000182	Pa×s	982.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356729&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

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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