Isophthalic acid, 2,5-dimethylphenyl heptyl ester

Inchi: InChI=1S/C23H28O4/c1-4-5-6-7-8-14-26-22(24)19-10-9-11-20(16-19)23(25)27-21-15-17

InchiKey: XZJIIVYLONGTOR-UHFFFAOYSA-N

Formula: C23H28O4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2C)c1

Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-129.13	kJ/mol	Joback Method
hf	-569.00	kJ/mol	Joback Method
hfus	47.81	kJ/mol	Joback Method
hvap	91.64	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.650		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2945.00		NIST Webbook
rinpol	2945.00		NIST Webbook
tb	946.52	K	Joback Method
tc	1169.97	K	Joback Method
tf	583.69	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.90	J/mol×K	946.52	Joback Method
cpg	1012.10	J/mol×K	1132.73	Joback Method
cpg	1003.30	J/mol×K	1095.49	Joback Method
cpg	993.22	J/mol×K	1058.25	Joback Method
cpg	981.81	J/mol×K	1021.00	Joback Method
cpg	969.05	J/mol×K	983.76	Joback Method
cpg	1019.64	J/mol×K	1169.97	Joback Method
dvisc	0.0000384	Pa×s	946.52	Joback Method

dvisc	0.0000481	Pa×s	886.05	Joback Method
dvisc	0.0000623	Pa×s	825.58	Joback Method
dvisc	0.0000840	Pa×s	765.11	Joback Method
dvisc	0.0001193	Pa×s	704.63	Joback Method
dvisc	0.0001810	Pa×s	644.16	Joback Method
dvisc	0.0002992	Pa×s	583.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344544&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