Isophthalic acid, heptyl 1-phenylpropyl ester

Inchi: InChI=1S/C24H30O4/c1-3-5-6-7-11-17-27-23(25)20-15-12-16-21(18-20)24(26)28-22(4-2
InchiKey: BCZMLXWJMITYDS-UHFFFAOYSA-N
Formula: C24H30O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OC(CC)c2ccccc2)c1
Mol. weight [g/mol]: 382.49

Physical Properties

Property code	Value	Unit	Source
gf	-103.89	kJ/mol	Joback Method
hf	-571.98	kJ/mol	Joback Method
hfus	47.66	kJ/mol	Joback Method
hvap	92.16	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	6.122		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2951.00		NIST Webbook
rinpol	2951.00		NIST Webbook
tb	959.00	K	Joback Method
tc	1183.19	K	Joback Method
tf	554.92	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.17	J/mol×K	959.00	Joback Method
cpg	1031.66	J/mol×K	996.37	Joback Method
cpg	1044.74	J/mol×K	1033.73	Joback Method
cpg	1056.47	J/mol×K	1071.10	Joback Method
cpg	1066.89	J/mol×K	1108.46	Joback Method
cpg	1076.05	J/mol×K	1145.83	Joback Method
cpg	1084.02	J/mol×K	1183.19	Joback Method
dvisc	0.0003715	Pa×s	554.92	Joback Method

dvisc	0.0001929	Pa×s	622.27	Joback Method
dvisc	0.0001139	Pa×s	689.61	Joback Method
dvisc	0.0000738	Pa×s	756.96	Joback Method
dvisc	0.0000514	Pa×s	824.31	Joback Method
dvisc	0.0000377	Pa×s	891.65	Joback Method
dvisc	0.0000290	Pa×s	959.00	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=U344553&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