Isophthalic acid, heptyl 2-propylphenyl ester

Inchi: InChI=1S/C24H30O4/c1-3-5-6-7-10-17-27-23(25)20-14-11-15-21(18-20)24(26)28-22-16-
InchiKey: NUSCMHUTPLLRKN-UHFFFAOYSA-N
Formula: C24H30O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2CCC)c1
Mol. weight [g/mol]: 382.49

Physical Properties

Property code	Value	Unit	Source
gf	-111.08	kJ/mol	Joback Method
hf	-578.17	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	93.21	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.986		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	2865.00		NIST Webbook
rinpol	2865.00		NIST Webbook
tb	964.42	K	Joback Method
tc	1187.99	K	Joback Method
tf	582.44	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.71	J/mol×K	964.42	Joback Method
cpg	1030.03	J/mol×K	1001.68	Joback Method
cpg	1042.95	J/mol×K	1038.94	Joback Method
cpg	1054.50	J/mol×K	1076.21	Joback Method
cpg	1064.74	J/mol×K	1113.47	Joback Method
cpg	1073.72	J/mol×K	1150.73	Joback Method
cpg	1081.47	J/mol×K	1187.99	Joback Method
dvisc	0.0003008	Pa×s	582.44	Joback Method

dvisc	0.0001730	Pa×s	646.10	Joback Method
dvisc	0.0001098	Pa×s	709.77	Joback Method
dvisc	0.0000752	Pa×s	773.43	Joback Method
dvisc	0.0000545	Pa×s	837.09	Joback Method
dvisc	0.0000413	Pa×s	900.76	Joback Method
dvisc	0.0000325	Pa×s	964.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356630&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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