Isophthalic acid, heptyl phenylethyl ester

Inchi: InChI=1S/C23H28O4/c1-2-3-4-5-9-16-26-22(24)20-13-10-14-21(18-20)23(25)27-17-15-1
InchiKey: SREBDSZSRALJCI-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-109.87	kJ/mol	Joback Method
hf	-546.06	kJ/mol	Joback Method
hfus	48.59	kJ/mol	Joback Method
hvap	90.32	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.213		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2991.00		NIST Webbook
rinpol	2991.00		NIST Webbook
tb	936.56	K	Joback Method
tc	1158.33	K	Joback Method
tf	558.65	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.00	J/mol×K	936.56	Joback Method
cpg	1015.97	J/mol×K	1121.37	Joback Method
cpg	1006.67	J/mol×K	1084.41	Joback Method
cpg	996.18	J/mol×K	1047.44	Joback Method
cpg	984.43	J/mol×K	1010.48	Joback Method
cpg	971.39	J/mol×K	973.52	Joback Method
cpg	1024.11	J/mol×K	1158.33	Joback Method
dvisc	0.0000368	Pa×s	936.56	Joback Method

dvisc	0.0000472	Pa×s	873.57	Joback Method
dvisc	0.0000628	Pa×s	810.59	Joback Method
dvisc	0.0000879	Pa×s	747.61	Joback Method
dvisc	0.0001307	Pa×s	684.62	Joback Method
dvisc	0.0002108	Pa×s	621.63	Joback Method
dvisc	0.0003786	Pa×s	558.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344338&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