Isophthalic acid, heptyl 1-naphthyl ester

Inchi: InChI=1S/C25H26O4/c1-2-3-4-5-8-17-28-24(26)20-13-9-14-21(18-20)25(27)29-23-16-10
InchiKey: FNSDBNDKQWWSRW-UHFFFAOYSA-N
Formula: C25H26O4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2cccc3ccccc23)c1
Mol. weight [g/mol]: 390.47

Physical Properties

Property code	Value	Unit	Source
gf	3.99	kJ/mol	Joback Method
hf	-407.74	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	97.07	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	6.186		Crippen Method
mcvol	311.010	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	3392.00		NIST Webbook
rinpol	3392.00		NIST Webbook
tb	1006.28	K	Joback Method
tc	1242.63	K	Joback Method
tf	626.41	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.44	J/mol×K	1006.28	Joback Method
cpg	1047.09	J/mol×K	1203.24	Joback Method
cpg	1038.20	J/mol×K	1163.84	Joback Method
cpg	1028.38	J/mol×K	1124.45	Joback Method
cpg	1017.54	J/mol×K	1085.06	Joback Method
cpg	1005.59	J/mol×K	1045.67	Joback Method
cpg	1055.13	J/mol×K	1242.63	Joback Method
dvisc	0.0000593	Pa×s	1006.28	Joback Method

dvisc	0.0000728	Pa×s	942.97	Joback Method
dvisc	0.0000920	Pa×s	879.66	Joback Method
dvisc	0.0001205	Pa×s	816.35	Joback Method
dvisc	0.0001653	Pa×s	753.03	Joback Method
dvisc	0.0002403	Pa×s	689.72	Joback Method
dvisc	0.0003766	Pa×s	626.41	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=U344691&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