Isophthalic acid, 1-naphthyl propyl ester

Inchi: InChI=1S/C21H18O4/c1-2-13-24-20(22)16-9-5-10-17(14-16)21(23)25-19-12-6-8-15-7-3-4
InchiKey: DAVSXTYHXUCMHT-UHFFFAOYSA-N
Formula: C21H18O4
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2cccc3ccccc23)c1
Mol. weight [g/mol]: 334.37

Physical Properties

Property code	Value	Unit	Source
gf	-29.69	kJ/mol	Joback Method
hf	-325.18	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	88.17	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	4.626		Crippen Method
mcvol	254.650	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	914.76	K	Joback Method
tc	1155.83	K	Joback Method
tf	581.33	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.45	J/mol×K	914.76	Joback Method
cpg	771.10	J/mol×K	954.94	Joback Method
cpg	782.55	J/mol×K	995.12	Joback Method
cpg	792.88	J/mol×K	1035.30	Joback Method
cpg	802.17	J/mol×K	1075.47	Joback Method
cpg	810.48	J/mol×K	1115.65	Joback Method
cpg	817.90	J/mol×K	1155.83	Joback Method
dvisc	0.0005468	Pa×s	581.33	Joback Method

dvisc	0.0003651	Pa×s	636.90	Joback Method
dvisc	0.0002601	Pa×s	692.47	Joback Method
dvisc	0.0001949	Pa×s	748.05	Joback Method
dvisc	0.0001519	Pa×s	803.62	Joback Method
dvisc	0.0001224	Pa×s	859.19	Joback Method
dvisc	0.0001012	Pa×s	914.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344686&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