Phthalic acid, heptyl hept-3-yl ester

Inchi: InChI=1S/C22H34O4/c1-4-7-9-10-13-17-25-21(23)19-15-11-12-16-20(19)22(24)26-18(6-
InchiKey: LQAQFECRFDVUAQ-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)CCCC
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-233.14	kJ/mol	Joback Method
hf	-767.23	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.939		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	886.56	K	Joback Method
tc	1090.83	K	Joback Method
tf	505.96	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.77	J/mol×K	886.56	Joback Method
cpg	1014.40	J/mol×K	920.61	Joback Method
cpg	1029.77	J/mol×K	954.65	Joback Method
cpg	1043.91	J/mol×K	988.70	Joback Method
cpg	1056.86	J/mol×K	1022.74	Joback Method
cpg	1068.64	J/mol×K	1056.79	Joback Method
cpg	1079.28	J/mol×K	1090.83	Joback Method
dvisc	0.0005411	Pa×s	505.96	Joback Method

dvisc	0.0002711	Pa×s	569.39	Joback Method
dvisc	0.0001560	Pa×s	632.83	Joback Method
dvisc	0.0000993	Pa×s	696.26	Joback Method
dvisc	0.0000682	Pa×s	759.69	Joback Method
dvisc	0.0000496	Pa×s	823.13	Joback Method
dvisc	0.0000377	Pa×s	886.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356991&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

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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