Phthalic acid, heptyl 4-methylhept-3-yl ester

Inchi: InChI=1S/C23H36O4/c1-5-8-9-10-13-17-26-22(24)19-15-11-12-16-20(19)23(25)27-21(7-
InchiKey: MCKQWWFLJRYLJL-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)CCC
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-227.16	kJ/mol	Joback Method
hf	-793.15	kJ/mol	Joback Method
hfus	47.51	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.185		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1109.63	kPa	Joback Method
rinpol	2492.00		NIST Webbook
tb	909.00	K	Joback Method
tc	1116.60	K	Joback Method
tf	502.23	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.99	J/mol×K	909.00	Joback Method
cpg	1130.24	J/mol×K	1082.00	Joback Method
cpg	1118.53	J/mol×K	1047.40	Joback Method
cpg	1105.58	J/mol×K	1012.80	Joback Method
cpg	1091.36	J/mol×K	978.20	Joback Method
cpg	1075.84	J/mol×K	943.60	Joback Method
cpg	1140.75	J/mol×K	1116.60	Joback Method
dvisc	0.0000298	Pa×s	909.00	Joback Method
dvisc	0.0000398	Pa×s	841.20	Joback Method

dvisc	0.0000559	Pa×s	773.41	Joback Method
dvisc	0.0000840	Pa×s	705.61	Joback Method
dvisc	0.0001374	Pa×s	637.82	Joback Method
dvisc	0.0002529	Pa×s	570.02	Joback Method
dvisc	0.0005486	Pa×s	502.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377942&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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