Phthalic acid, hept-4-yl nonyl ester

Inchi: InChI=1S/C24H38O4/c1-4-7-8-9-10-11-14-19-27-23(25)21-17-12-13-18-22(21)24(26)28-
InchiKey: ZNIUKIXXQSSLPW-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CCC)CCC
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-216.30	kJ/mol	Joback Method
hf	-808.51	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.720		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1036.57	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	932.32	K	Joback Method
tc	1142.37	K	Joback Method
tf	528.50	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.86	J/mol×K	932.32	Joback Method
cpg	1136.88	J/mol×K	967.33	Joback Method
cpg	1152.52	J/mol×K	1002.34	Joback Method
cpg	1166.82	J/mol×K	1037.34	Joback Method
cpg	1179.81	J/mol×K	1072.35	Joback Method
cpg	1191.53	J/mol×K	1107.36	Joback Method
cpg	1202.02	J/mol×K	1142.37	Joback Method
dvisc	0.0004292	Pa×s	528.50	Joback Method

dvisc	0.0002108	Pa×s	595.80	Joback Method
dvisc	0.0001196	Pa×s	663.11	Joback Method
dvisc	0.0000753	Pa×s	730.41	Joback Method
dvisc	0.0000513	Pa×s	797.71	Joback Method
dvisc	0.0000371	Pa×s	865.02	Joback Method
dvisc	0.0000281	Pa×s	932.32	Joback Method

Sources

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=U356790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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