Adipic acid, octyl 2-propylphenyl ester

Inchi: InChI=1S/C23H36O4/c1-3-5-6-7-8-13-19-26-22(24)17-11-12-18-23(25)27-21-16-10-9-15
InchiKey: QXXIACXKVCWHPY-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCOC(=O)CCCCC(=O)Oc1ccccc1CCC
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-222.28	kJ/mol	Joback Method
hf	-782.59	kJ/mol	Joback Method
hfus	54.55	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.009		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2668.00		NIST Webbook
rinpol	2668.00		NIST Webbook
tb	909.88	K	Joback Method
tc	1115.88	K	Joback Method
tf	532.23	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.08	J/mol×K	909.88	Joback Method
cpg	1074.86	J/mol×K	944.21	Joback Method
cpg	1090.35	J/mol×K	978.55	Joback Method
cpg	1104.59	J/mol×K	1012.88	Joback Method
cpg	1117.59	J/mol×K	1047.21	Joback Method
cpg	1129.40	J/mol×K	1081.55	Joback Method
cpg	1140.05	J/mol×K	1115.88	Joback Method
dvisc	0.0004311	Pa×s	532.23	Joback Method

dvisc	0.0002285	Pa×s	595.17	Joback Method
dvisc	0.0001367	Pa×s	658.11	Joback Method
dvisc	0.0000895	Pa×s	721.06	Joback Method
dvisc	0.0000627	Pa×s	784.00	Joback Method
dvisc	0.0000463	Pa×s	846.94	Joback Method
dvisc	0.0000357	Pa×s	909.88	Joback Method

Sources

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=U353831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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