Adipic acid, ethyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C21H24O5/c1-2-24-20(22)13-6-7-14-21(23)25-16-17-9-8-12-19(15-17)26-18-1
InchiKey: WHQWPJWYJCCKHC-UHFFFAOYSA-N
Formula: C21H24O5
SMILES: CCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 356.41

Physical Properties

Property code	Value	Unit	Source
gf	-231.71	kJ/mol	Joback Method
hf	-637.00	kJ/mol	Joback Method
hfus	44.60	kJ/mol	Joback Method
hvap	88.28	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.646		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2692.00		NIST Webbook
tb	913.22	K	Joback Method
tc	1135.44	K	Joback Method
tf	558.34	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.73	J/mol×K	913.22	Joback Method
cpg	920.56	J/mol×K	1098.41	Joback Method
cpg	912.49	J/mol×K	1061.37	Joback Method
cpg	903.09	J/mol×K	1024.33	Joback Method
cpg	892.35	J/mol×K	987.29	Joback Method
cpg	880.24	J/mol×K	950.26	Joback Method
cpg	927.34	J/mol×K	1135.44	Joback Method
dvisc	0.0000366	Pa×s	913.22	Joback Method
dvisc	0.0000465	Pa×s	854.07	Joback Method

dvisc	0.0000612	Pa×s	794.93	Joback Method
dvisc	0.0000843	Pa×s	735.78	Joback Method
dvisc	0.0001227	Pa×s	676.63	Joback Method
dvisc	0.0001920	Pa×s	617.49	Joback Method
dvisc	0.0003303	Pa×s	558.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353810&Units=SI

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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