Adipic acid, isobutyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H28O5/c1-18(2)16-26-22(24)13-6-7-14-23(25)27-17-19-9-8-12-21(15-19)2
InchiKey: JVWYSYCCKHZVMA-UHFFFAOYSA-N
Formula: C23H28O5
SMILES: CC(C)COC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 384.47

Physical Properties

Property code	Value	Unit	Source
gf	-217.31	kJ/mol	Joback Method
hf	-683.56	kJ/mol	Joback Method
hfus	46.26	kJ/mol	Joback Method
hvap	92.34	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.282		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2827.00		NIST Webbook
tb	958.54	K	Joback Method
tc	1183.12	K	Joback Method
tf	565.88	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.98	J/mol×K	958.54	Joback Method
cpg	1037.98	J/mol×K	1145.69	Joback Method
cpg	1030.27	J/mol×K	1108.26	Joback Method
cpg	1021.15	J/mol×K	1070.83	Joback Method
cpg	1010.58	J/mol×K	1033.40	Joback Method
cpg	998.54	J/mol×K	995.97	Joback Method
cpg	1044.31	J/mol×K	1183.12	Joback Method
dvisc	0.0000249	Pa×s	958.54	Joback Method
dvisc	0.0000323	Pa×s	893.10	Joback Method

dvisc	0.0000436	Pa×s	827.65	Joback Method
dvisc	0.0000619	Pa×s	762.21	Joback Method
dvisc	0.0000940	Pa×s	696.77	Joback Method
dvisc	0.0001556	Pa×s	631.32	Joback Method
dvisc	0.0002894	Pa×s	565.88	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=U353812&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