Adipic acid, butyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H28O5/c1-2-3-16-26-22(24)14-7-8-15-23(25)27-18-19-10-9-13-21(17-19)2
InchiKey: FNYVNVFBTDWZPE-UHFFFAOYSA-N
Formula: C23H28O5
SMILES: CCCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 384.47

Physical Properties

Property code	Value	Unit	Source
gf	-214.87	kJ/mol	Joback Method
hf	-678.28	kJ/mol	Joback Method
hfus	49.78	kJ/mol	Joback Method
hvap	92.73	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.426		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2873.00		NIST Webbook
rinpol	2873.00		NIST Webbook
tb	958.98	K	Joback Method
tc	1182.01	K	Joback Method
tf	580.88	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.53	J/mol×K	958.98	Joback Method
cpg	998.05	J/mol×K	996.15	Joback Method
cpg	1010.09	J/mol×K	1033.32	Joback Method
cpg	1020.69	J/mol×K	1070.49	Joback Method
cpg	1029.87	J/mol×K	1107.66	Joback Method
cpg	1037.67	J/mol×K	1144.84	Joback Method
cpg	1044.12	J/mol×K	1182.01	Joback Method
dvisc	0.0002656	Pa×s	580.88	Joback Method

dvisc	0.0001511	Pa×s	643.90	Joback Method
dvisc	0.0000950	Pa×s	706.91	Joback Method
dvisc	0.0000644	Pa×s	769.93	Joback Method
dvisc	0.0000464	Pa×s	832.95	Joback Method
dvisc	0.0000349	Pa×s	895.96	Joback Method
dvisc	0.0000273	Pa×s	958.98	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=U353813&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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