

Sebacic acid, butyl 3-phenylpropyl ester

Inchi:	InChI=1S/C23H36O4/c1-2-3-19-26-22(24)17-11-6-4-5-7-12-18-23(25)27-20-13-16-21-14
InchiKey:	WUVORUXRPVVZML-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-212.65	kJ/mol	Joback Method
hf	-771.12	kJ/mol	Joback Method
hfus	54.94	kJ/mol	Joback Method
hvap	87.38	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.627		Crippen Method
mvol	326.050	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpol	2875.00		NIST Webbook
tb	904.90	K	Joback Method
tc	1109.91	K	Joback Method
tf	519.71	K	Joback Method
vc	1.264	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.61	J/molxK	904.90	Joback Method
cpg	1130.59	J/molxK	1075.74	Joback Method
cpg	1118.60	J/molxK	1041.57	Joback Method
cpg	1105.44	J/molxK	1007.40	Joback Method
cpg	1091.08	J/molxK	973.24	Joback Method
cpg	1075.49	J/molxK	939.07	Joback Method
cpg	1141.46	J/molxK	1109.91	Joback Method
dvisc	0.0000350	Paxs	904.90	Joback Method
dvisc	0.0000461	Paxs	840.70	Joback Method

dvisc	0.0000634	Paxs	776.50	Joback Method
dvisc	0.0000925	Paxs	712.30	Joback Method
dvisc	0.0001452	Paxs	648.11	Joback Method
dvisc	0.0002518	Paxs	583.91	Joback Method
dvisc	0.0005005	Paxs	519.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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