

Sebacic acid, isobutyl 4-methoxybenzyl ester

Inchi:	InChI=1S/C22H34O5/c1-18(2)16-26-21(23)10-8-6-4-5-7-9-11-22(24)27-17-19-12-14-20(2)
InchiKey:	OAYKJJBCVAKERL-UHFFFAOYSA-N
Formula:	C22H34O5
SMILES:	COc1ccc(COC(=O)CCCCCCCCC(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	378.50

Physical Properties

Property code	Value	Unit	Source
gf	-338.14	kJ/mol	Joback Method
hf	-899.45	kJ/mol	Joback Method
hfus	49.63	kJ/mol	Joback Method
hvap	87.84	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.058		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpola	2842.00		NIST Webbook
tb	908.98	K	Joback Method
tc	1115.86	K	Joback Method
tf	528.19	K	Joback Method
vc	1.220	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.47	J/molxK	908.98	Joback Method
cpg	1043.51	J/molxK	943.46	Joback Method
cpg	1058.17	J/molxK	977.94	Joback Method
cpg	1071.48	J/molxK	1012.42	Joback Method
cpg	1083.45	J/molxK	1046.90	Joback Method
cpg	1094.10	J/molxK	1081.38	Joback Method
cpg	1103.44	J/molxK	1115.86	Joback Method
dvisc	0.0003727	Paxs	528.19	Joback Method
dvisc	0.0001922	Paxs	591.65	Joback Method

dvisc	0.0001127	Paxs	655.12	Joback Method
dvisc	0.0000726	Paxs	718.59	Joback Method
dvisc	0.0000503	Paxs	782.05	Joback Method
dvisc	0.0000367	Paxs	845.51	Joback Method
dvisc	0.0000281	Paxs	908.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354362&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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