

Sebacic acid, isobutyl 5-methoxy-3-phenylpentyl ester

Inchi:	InChI=1S/C26H42O5/c1-22(2)21-31-26(28)16-12-7-5-4-6-11-15-25(27)30-20-18-24(17-1
InchiKey:	QZONAKBACCLWBY-UHFFFAOYSA-N
Formula:	C26H42O5
SMILES:	COCCC(CCOC(=O)CCCCCCCCC(=O)OCC(C)C)c1ccccc1
Mol. weight [g/mol]:	434.61

Physical Properties

Property code	Value	Unit	Source
gf	-297.27	kJ/mol	Joback Method
hf	-975.82	kJ/mol	Joback Method
hfus	56.85	kJ/mol	Joback Method
hvap	95.69	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	6.060		Crippen Method
mcvol	374.190	ml/mol	McGowan Method
pc	922.74	kPa	Joback Method
rinqol	3043.00		NIST Webbook
tb	995.08	K	Joback Method
tc	1218.85	K	Joback Method
tf	545.75	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.47	J/molxK	995.08	Joback Method
cpg	1291.21	J/molxK	1032.38	Joback Method
cpg	1306.22	J/molxK	1069.67	Joback Method
cpg	1319.53	J/molxK	1106.97	Joback Method
cpg	1331.20	J/molxK	1144.26	Joback Method
cpg	1341.27	J/molxK	1181.56	Joback Method
cpg	1349.77	J/molxK	1218.85	Joback Method
dvisc	0.0002958	Paxs	545.75	Joback Method
dvisc	0.0001298	Paxs	620.64	Joback Method

dvisc	0.0000680	Paxs	695.53	Joback Method
dvisc	0.0000404	Paxs	770.41	Joback Method
dvisc	0.0000263	Paxs	845.30	Joback Method
dvisc	0.0000184	Paxs	920.19	Joback Method
dvisc	0.0000136	Paxs	995.08	Joback Method

Sources

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=U355481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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