

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

Inchi:	InChI=1S/C21H40O5/c1-18(2)17-26-21(23)12-10-8-6-5-7-9-11-20(22)25-16-14-19(3)13-
InchiKey:	SSUNGIINBJHCPC-UHFFFAOYSA-N
Formula:	C21H40O5
SMILES:	COCCC(C)CCOC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	372.54

Physical Properties

Property code	Value	Unit	Source
gf	-451.78	kJ/mol	Joback Method
hf	-1109.15	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.912		Crippen Method
mvol	327.500	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	854.00	K	Joback Method
tc	1046.11	K	Joback Method
tf	462.98	K	Joback Method
vc	1.266	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.08	J/molxK	854.00	Joback Method
cpg	1081.57	J/molxK	886.02	Joback Method
cpg	1098.82	J/molxK	918.04	Joback Method
cpg	1114.82	J/molxK	950.06	Joback Method
cpg	1129.61	J/molxK	982.07	Joback Method
cpg	1143.18	J/molxK	1014.09	Joback Method
cpg	1155.54	J/molxK	1046.11	Joback Method
dvisc	0.0006967	Paxs	462.98	Joback Method

dvisc	0.0002952	Paxs	528.15	Joback Method
dvisc	0.0001510	Paxs	593.32	Joback Method
dvisc	0.0000882	Paxs	658.49	Joback Method
dvisc	0.0000568	Paxs	723.66	Joback Method
dvisc	0.0000393	Paxs	788.83	Joback Method
dvisc	0.0000288	Paxs	854.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355500&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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