

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

Inchi:	InChI=1S/C23H44O5/c1-20(2)12-11-17-27-22(24)13-9-7-5-6-8-10-14-23(25)28-19-16-21
InchiKey:	IMIARUQZYSFUQV-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	COCCC(C)CCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	400.59

Physical Properties

Property code	Value	Unit	Source
gf	-434.94	kJ/mol	Joback Method
hf	-1150.43	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	86.74	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.692		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpola	2711.00		NIST Webbook
tb	899.76	K	Joback Method
tc	1101.93	K	Joback Method
tf	485.52	K	Joback Method
vc	1.377	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.52	J/molxK	899.76	Joback Method
cpg	1206.77	J/molxK	933.46	Joback Method
cpg	1224.57	J/molxK	967.15	Joback Method
cpg	1240.93	J/molxK	1000.85	Joback Method
cpg	1255.86	J/molxK	1034.54	Joback Method
cpg	1269.40	J/molxK	1068.24	Joback Method
cpg	1281.54	J/molxK	1101.93	Joback Method
dvisc	0.0005368	Paxs	485.52	Joback Method
dvisc	0.0002239	Paxs	554.56	Joback Method

dvisc	0.0001133	Paxs	623.60	Joback Method
dvisc	0.0000657	Paxs	692.64	Joback Method
dvisc	0.0000421	Paxs	761.68	Joback Method
dvisc	0.0000290	Paxs	830.72	Joback Method
dvisc	0.0000212	Paxs	899.76	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=U355503&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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