

Sebacic acid, isohexyl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C21H40O4/c1-17(2)13-12-16-24-20(22)14-10-8-6-7-9-11-15-21(23)25-19(5)18
InchiKey:	FSNCWZMNEZKZPF-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-349.22	kJ/mol	Joback Method
hf	-982.21	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.674		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinsol	2364.00		NIST Webbook
tb	831.14	K	Joback Method
tc	1020.11	K	Joback Method
tf	425.75	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.67	J/molxK	831.14	Joback Method
cpg	1114.48	J/molxK	988.62	Joback Method
cpg	1100.16	J/molxK	957.12	Joback Method
cpg	1084.74	J/molxK	925.63	Joback Method
cpg	1068.19	J/molxK	894.13	Joback Method
cpg	1050.51	J/molxK	862.64	Joback Method
cpg	1127.72	J/molxK	1020.11	Joback Method
dvisc	0.0000355	Paxs	831.14	Joback Method
dvisc	0.0000496	Paxs	763.58	Joback Method

dvisc	0.0000739	Paxs	696.01	Joback Method
dvisc	0.0001201	Paxs	628.44	Joback Method
dvisc	0.0002191	Paxs	560.88	Joback Method
dvisc	0.0004714	Paxs	493.32	Joback Method
dvisc	0.0012935	Paxs	425.75	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=U355561&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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