

Sebacic acid, isohexyl 4-octyl ester

Inchi:	InChI=1S/C24H46O4/c1-5-7-17-22(15-6-2)28-24(26)19-13-11-9-8-10-12-18-23(25)27-20
InchiKey:	XOXFWNQGSJMBX-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCC(CCC)OC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	398.62

Physical Properties

Property code	Value	Unit	Source
gf	-321.52	kJ/mol	Joback Method
hf	-1038.85	kJ/mol	Joback Method
hfus	56.44	kJ/mol	Joback Method
hvap	86.55	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.989		Crippen Method
mvol	363.900	ml/mol	McGowan Method
pc	857.97	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	900.22	K	Joback Method
tc	1102.59	K	Joback Method
tf	474.56	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.42	J/molxK	900.22	Joback Method
cpg	1304.81	J/molxK	1068.86	Joback Method
cpg	1290.22	J/molxK	1035.14	Joback Method
cpg	1274.32	J/molxK	1001.41	Joback Method
cpg	1257.07	J/molxK	967.68	Joback Method
cpg	1238.45	J/molxK	933.95	Joback Method
cpg	1318.12	J/molxK	1102.59	Joback Method
dvisc	0.0000246	Paxs	900.22	Joback Method

dvisc	0.0000339	Paxs	829.28	Joback Method
dvisc	0.0000496	Paxs	758.33	Joback Method
dvisc	0.0000786	Paxs	687.39	Joback Method
dvisc	0.0001385	Paxs	616.45	Joback Method
dvisc	0.0002826	Paxs	545.50	Joback Method
dvisc	0.0007142	Paxs	474.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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