

Sebacic acid, 2-methylbenzyl nonyl ester

Inchi: InChI=1S/C27H44O4/c1-3-4-5-6-9-12-17-22-30-26(28)20-13-10-7-8-11-14-21-27(29)31-2
InchiKey: NCLKJRIUTLFCJX-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1C
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-188.60	kJ/mol	Joback Method
hf	-865.15	kJ/mol	Joback Method
hfus	64.91	kJ/mol	Joback Method
hvap	96.95	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	7.453		Crippen Method
mvol	382.410	ml/mol	McGowan Method
pc	864.04	kPa	Joback Method
rinpol	3143.00		NIST Webbook
rinpol	3143.00		NIST Webbook
tb	1001.40	K	Joback Method
tc	1228.17	K	Joback Method
tf	577.31	K	Joback Method
vc	1.488	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.45	J/molxK	1001.40	Joback Method
cpg	1324.35	J/molxK	1039.19	Joback Method
cpg	1340.59	J/molxK	1076.99	Joback Method
cpg	1355.23	J/molxK	1114.78	Joback Method
cpg	1368.34	J/molxK	1152.58	Joback Method
cpg	1379.97	J/molxK	1190.37	Joback Method
cpg	1390.19	J/molxK	1228.17	Joback Method
dvisc	0.0002685	Paxs	577.31	Joback Method

dvisc	0.0001367	Paxs	647.99	Joback Method
dvisc	0.0000795	Paxs	718.67	Joback Method
dvisc	0.0000510	Paxs	789.36	Joback Method
dvisc	0.0000351	Paxs	860.04	Joback Method
dvisc	0.0000256	Paxs	930.72	Joback Method
dvisc	0.0000195	Paxs	1001.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380720&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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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