

Sebacic acid, 2-methylbenzyl octyl ester

Inchi:	InChI=1S/C26H42O4/c1-3-4-5-6-11-16-21-29-25(27)19-12-9-7-8-10-13-20-26(28)30-22-2
InchiKey:	SDOJXLXXFYSAFZ-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)OCc1ccccc1C
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-197.02	kJ/mol	Joback Method
hf	-844.51	kJ/mol	Joback Method
hfus	62.32	kJ/mol	Joback Method
hvap	94.72	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.063		Crippen Method
mvol	368.320	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	3051.00		NIST Webbook
rinpol	3051.00		NIST Webbook
tb	978.52	K	Joback Method
tc	1198.52	K	Joback Method
tf	566.04	K	Joback Method
vc	1.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.68	J/molxK	978.52	Joback Method
cpg	1316.64	J/molxK	1161.85	Joback Method
cpg	1304.93	J/molxK	1125.19	Joback Method
cpg	1291.83	J/molxK	1088.52	Joback Method
cpg	1277.29	J/molxK	1051.85	Joback Method
cpg	1261.26	J/molxK	1015.19	Joback Method
cpg	1327.00	J/molxK	1198.52	Joback Method
dvisc	0.0000228	Paxs	978.52	Joback Method

dvisc	0.0000298	Paxs	909.77	Joback Method
dvisc	0.0000407	Paxs	841.03	Joback Method
dvisc	0.0000589	Paxs	772.28	Joback Method
dvisc	0.0000914	Paxs	703.53	Joback Method
dvisc	0.0001561	Paxs	634.79	Joback Method
dvisc	0.0003036	Paxs	566.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380719&Units=SI

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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