

Sebacic acid, di(2-methylbenzyl) ester

Inchi:	InChI=1S/C26H34O4/c1-21-13-9-11-15-23(21)19-29-25(27)17-7-5-3-4-6-8-18-26(28)30-2
InchiKey:	WLWZPKIVZLSVEU-UHFFFAOYSA-N
Formula:	C26H34O4
SMILES:	Cc1cccc1COC(=O)CCCCCCCCC(=O)OCc1cccc1C
Mol. weight [g/mol]:	410.55

Physical Properties

Property code	Value	Unit	Source
gf	-94.24	kJ/mol	Joback Method
hf	-619.45	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	97.66	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.211		Crippen Method
mvol	344.560	ml/mol	McGowan Method
pc	1118.56	kPa	Joback Method
rinpol	3151.00		NIST Webbook
rinpol	3151.00		NIST Webbook
tb	1010.18	K	Joback Method
tc	1238.38	K	Joback Method
tf	604.98	K	Joback Method
vc	1.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.73	J/molxK	1010.18	Joback Method
cpg	1151.16	J/molxK	1048.21	Joback Method
cpg	1164.09	J/molxK	1086.25	Joback Method
cpg	1175.57	J/molxK	1124.28	Joback Method
cpg	1185.67	J/molxK	1162.32	Joback Method
cpg	1194.43	J/molxK	1200.35	Joback Method
cpg	1201.91	J/molxK	1238.38	Joback Method
dvisc	0.0002402	Paxs	604.98	Joback Method

dvisc	0.0001352	Paxs	672.51	Joback Method
dvisc	0.0000846	Paxs	740.05	Joback Method
dvisc	0.0000572	Paxs	807.58	Joback Method
dvisc	0.0000411	Paxs	875.11	Joback Method
dvisc	0.0000310	Paxs	942.65	Joback Method
dvisc	0.0000242	Paxs	1010.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380723&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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