

Sebacic acid, 2-methylbenzyl propyl ester

Inchi:	InChI=1S/C21H32O4/c1-3-16-24-20(22)14-8-6-4-5-7-9-15-21(23)25-17-19-13-11-10-12-
InchiKey:	JFYSSNBCDAMSPM-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1C
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-239.12	kJ/mol	Joback Method
hf	-741.31	kJ/mol	Joback Method
hfus	49.37	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.112		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1252.15	kPa	Joback Method
rinpol	2573.00		NIST Webbook
rinpol	2573.00		NIST Webbook
tb	864.12	K	Joback Method
tc	1065.34	K	Joback Method
tf	509.69	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.16	J/molxK	864.12	Joback Method
cpg	953.50	J/molxK	897.66	Joback Method
cpg	968.67	J/molxK	931.19	Joback Method
cpg	982.68	J/molxK	964.73	Joback Method
cpg	995.57	J/molxK	998.27	Joback Method
cpg	1007.37	J/molxK	1031.80	Joback Method
cpg	1018.08	J/molxK	1065.34	Joback Method
dvisc	0.0005353	Paxs	509.69	Joback Method

dvisc	0.0002901	Paxs	568.76	Joback Method
dvisc	0.0001764	Paxs	627.83	Joback Method
dvisc	0.0001169	Paxs	686.90	Joback Method
dvisc	0.0000826	Paxs	745.98	Joback Method
dvisc	0.0000615	Paxs	805.05	Joback Method
dvisc	0.0000476	Paxs	864.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380713&Units=SI
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

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
mccvol:	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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