

Sebacic acid, butyl 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C22H34O4/c1-4-5-17-25-21(23)15-10-8-6-7-9-11-16-22(24)26-20-14-12-13-18
InchiKey:	YXOSBYRYHFBYCM-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-240.33	kJ/mol	Joback Method
hf	-773.42	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	86.48	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.673		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinqol	2738.00		NIST Webbook
tb	891.98	K	Joback Method
tc	1096.12	K	Joback Method
tf	533.48	K	Joback Method
vc	1.208	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.72	J/molxK	891.98	Joback Method
cpg	1013.19	J/molxK	926.00	Joback Method
cpg	1028.42	J/molxK	960.03	Joback Method
cpg	1042.43	J/molxK	994.05	Joback Method
cpg	1055.25	J/molxK	1028.08	Joback Method
cpg	1066.89	J/molxK	1062.10	Joback Method
cpg	1077.39	J/molxK	1096.12	Joback Method
dvisc	0.0004177	Paxs	533.48	Joback Method
dvisc	0.0002348	Paxs	593.23	Joback Method

dvisc	0.0001467	Paxs	652.98	Joback Method
dvisc	0.0000992	Paxs	712.73	Joback Method
dvisc	0.0000712	Paxs	772.48	Joback Method
dvisc	0.0000537	Paxs	832.23	Joback Method
dvisc	0.0000420	Paxs	891.98	Joback Method

Sources

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=U355206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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