

Sebacic acid, isobutyl 4-isopropylphenyl ester

Inchi: InChI=1S/C23H36O4/c1-18(2)17-26-22(24)11-9-7-5-6-8-10-12-23(25)27-21-15-13-20(14)
InchiKey: BXOMEYXBLFEJAH-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-227.16	kJ/mol	Joback Method
hf	-793.15	kJ/mol	Joback Method
hfus	47.51	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.035		Crippen Method
mvol	326.050	ml/mol	McGowan Method
pc	1109.63	kPa	Joback Method
rinpol	2778.00		NIST Webbook
rinpol	2778.00		NIST Webbook
tb	909.00	K	Joback Method
tc	1116.60	K	Joback Method
tf	502.23	K	Joback Method
vc	1.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.99	J/molxK	909.00	Joback Method
cpg	1130.24	J/molxK	1082.00	Joback Method
cpg	1118.53	J/molxK	1047.40	Joback Method
cpg	1105.58	J/molxK	1012.80	Joback Method
cpg	1091.36	J/molxK	978.20	Joback Method
cpg	1075.84	J/molxK	943.60	Joback Method
cpg	1140.75	J/molxK	1116.60	Joback Method
dvisc	0.0000298	Paxs	909.00	Joback Method

dvisc	0.0000398	Paxs	841.20	Joback Method
dvisc	0.0000559	Paxs	773.41	Joback Method
dvisc	0.0000840	Paxs	705.61	Joback Method
dvisc	0.0001374	Paxs	637.82	Joback Method
dvisc	0.0002529	Paxs	570.02	Joback Method
dvisc	0.0005486	Paxs	502.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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