

Succinic acid, 3,5-dimethylphenyl 2-methoxyethyl ester

Inchi:	InChI=1S/C15H20O5/c1-11-8-12(2)10-13(9-11)20-15(17)5-4-14(16)19-7-6-18-3/h8-10H,4
InchiKey:	PKFZAKXEWDWPA-UHFFFAOYSA-N
Formula:	C15H20O5
SMILES:	COCCOC(=O)CCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	280.32

Physical Properties

Property code	Value	Unit	Source
gf	-404.27	kJ/mol	Joback Method
hf	-761.16	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	73.31	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.179		Crippen Method
mvol	219.200	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rmpol	2098.00		NIST Webbook
rmpol	2098.00		NIST Webbook
tb	754.24	K	Joback Method
tc	957.56	K	Joback Method
tf	476.82	K	Joback Method
vc	0.834	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.00	J/molxK	754.24	Joback Method
cpg	634.33	J/molxK	788.13	Joback Method
cpg	647.72	J/molxK	822.01	Joback Method
cpg	660.15	J/molxK	855.90	Joback Method
cpg	671.62	J/molxK	889.79	Joback Method
cpg	682.11	J/molxK	923.67	Joback Method
cpg	691.62	J/molxK	957.56	Joback Method
dvisc	0.0005654	Paxs	476.82	Joback Method

dvisc	0.0003549	Paxs	523.06	Joback Method
dvisc	0.0002402	Paxs	569.29	Joback Method
dvisc	0.0001725	Paxs	615.53	Joback Method
dvisc	0.0001297	Paxs	661.77	Joback Method
dvisc	0.0001012	Paxs	708.00	Joback Method
dvisc	0.0000814	Paxs	754.24	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=U360726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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