Succinic acid, butyl (5-ethyl-1,3-dioxan-5-yl)methyl ester

Inchi: InChI=1S/C15H26O6/c1-3-5-8-20-13(16)6-7-14(17)21-11-15(4-2)9-18-12-19-10-15/h3-12

InchiKey: LBMOYNWVGASVGG-UHFFFAOYSA-N

Formula: C15H26O6

SMILES: CCCCOC(=O)CCC(=O)OCC1(CC)COCOC1

Mol. weight [g/mol]: 302.36

Physical Properties

Property code	Value	Unit	Source
gf	-545.70	kJ/mol	Joback Method
hf	-1036.97	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	75.59	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.054		Crippen Method
mcvol	237.970	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	768.87	K	Joback Method
tc	971.22	K	Joback Method
tf	487.55	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.71	J/mol×K	768.87	Joback Method
cpg	751.82	J/mol×K	802.60	Joback Method
cpg	768.20	J/mol×K	836.32	Joback Method
cpg	783.92	J/mol×K	870.05	Joback Method
cpg	799.05	J/mol×K	903.77	Joback Method
cpg	813.67	J/mol×K	937.50	Joback Method
cpg	827.86	J/mol×K	971.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382205&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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