1,3-Cyclobutanediol, 2,4-diethyl-2,4-dimethyl-, dipelargonate

Inchi: InChI=1S/C28H52O4/c1-7-11-13-15-17-19-21-23(29)31-25-27(5,9-3)26(28(25,6)10-4)32-
InchiKey: YWIXAQMTRDSEPQ-UHFFFAOYSA-N
Formula: C28H52O4
SMILES: CCCCCCCCC(=O)OC1C(C)(CC)C(OC(=O)CCCCCCCC)C1(C)CC
Mol. weight [g/mol]: 452.71
CAS: 105476-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-268.42	kJ/mol	Joback Method
hf	-1074.75	kJ/mol	Joback Method
hfus	60.50	kJ/mol	Joback Method
hvap	93.09	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	8.157		Crippen Method
mcvol	409.400	ml/mol	McGowan Method
pc	743.26	kPa	Joback Method
tb	990.10	K	Joback Method
tc	1215.43	K	Joback Method
tf	599.14	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1486.88	J/mol×K	990.10	Joback Method
cpg	1517.96	J/mol×K	1027.66	Joback Method
cpg	1549.26	J/mol×K	1065.21	Joback Method
cpg	1581.02	J/mol×K	1102.77	Joback Method
cpg	1613.48	J/mol×K	1140.32	Joback Method
cpg	1646.91	J/mol×K	1177.88	Joback Method
cpg	1681.54	J/mol×K	1215.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105476844&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume