1,3-Cyclobutanediol, 2,2,4,4-tetramethyl-, nonanoate, 2-ethylhexanoate

Inchi: InChI=1S/C25H46O4/c1-8-11-13-14-15-16-18-20(26)28-22-24(4,5)23(25(22,6)7)29-21(2

InchiKey: WKCWUKVEWJJOQL-UHFFFAOYSA-N

Formula: C25H46O4

SMILES: CCCCCCCCC(=O)OC1C(C)(C)C(OC(=O)C(CC)CCCC)C1(C)C

Mol. weight [g/mol]: 410.63

CAS: 116401-23-1

Physical Properties

Property code	Value	Unit	Source
gf	-296.12	kJ/mol	Joback Method
hf	-1018.11	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.843		Crippen Method
mcvol	367.130	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
tb	921.02	K	Joback Method
tc	1127.99	K	Joback Method
tf	550.33	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1280.90	J/mol×K	921.02	Joback Method
cpg	1307.12	J/mol×K	955.52	Joback Method
cpg	1333.25	J/mol×K	990.01	Joback Method
cpg	1359.48	J/mol×K	1024.51	Joback Method
cpg	1386.00	J/mol×K	1059.00	Joback Method
cpg	1412.98	J/mol×K	1093.50	Joback Method
cpg	1440.60	J/mol×K	1127.99	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=C116401231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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