1,2-Cyclohexanedicarboxylic acid, 2-adamantyl butyl ester

Inchi: InChI=1S/C22H34O4/c1-2-3-8-25-21(23)18-6-4-5-7-19(18)22(24)26-20-16-10-14-9-15(12

InchiKey: RBQIYDCEYQKHFC-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)OC1C2CC3CC(C2)CC1C3

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-162.01	kJ/mol	Joback Method
hf	-781.47	kJ/mol	Joback Method
hfus	45.66	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.504		Crippen Method
mcvol	292.280	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2682.00		NIST Webbook
rinpol	2682.00		NIST Webbook
tb	885.37	K	Joback Method
tc	1105.67	K	Joback Method
tf	526.98	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.74	J/mol×K	885.37	Joback Method
cpg	1144.86	J/mol×K	1068.95	Joback Method
cpg	1129.73	J/mol×K	1032.24	Joback Method
cpg	1113.34	J/mol×K	995.52	Joback Method
cpg	1095.61	J/mol×K	958.80	Joback Method
cpg	1076.44	J/mol×K	922.09	Joback Method
cpg	1158.84	J/mol×K	1105.67	Joback Method
dvisc	0.0020184	Pa×s	885.37	Joback Method

dvisc	0.0022200	Pa×s	825.64	Joback Method
dvisc	0.0024784	Pa×s	765.91	Joback Method
dvisc	0.0028189	Pa×s	706.17	Joback Method
dvisc	0.0032833	Pa×s	646.44	Joback Method
dvisc	0.0039449	Pa×s	586.71	Joback Method
dvisc	0.0049412	Pa×s	526.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339768&Units=SI

Legend

cpg:	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:	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