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

Inchi: InChI=1S/C25H40O4/c1-2-3-4-5-8-11-28-24(26)21-9-6-7-10-22(21)25(27)29-23-19-13-17

InchiKey: PRINMDXCNOUEAK-UHFFFAOYSA-N

Formula: C25H40O4

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

Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-136.75	kJ/mol	Joback Method
hf	-843.39	kJ/mol	Joback Method
hfus	53.43	kJ/mol	Joback Method
hvap	88.97	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.674		Crippen Method
mcvol	334.550	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	2975.00		NIST Webbook
rinpol	2975.00		NIST Webbook
tb	954.01	K	Joback Method
tc	1175.02	K	Joback Method
tf	560.79	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.82	J/mol×K	954.01	Joback Method
cpg	1265.33	J/mol×K	990.85	Joback Method
cpg	1284.31	J/mol×K	1027.68	Joback Method
cpg	1301.88	J/mol×K	1064.52	Joback Method
cpg	1318.14	J/mol×K	1101.35	Joback Method
cpg	1333.19	J/mol×K	1138.19	Joback Method
cpg	1347.15	J/mol×K	1175.02	Joback Method
dvisc	0.0043964	Pa×s	560.79	Joback Method

dvisc	0.0033555	Pa×s	626.33	Joback Method
dvisc	0.0026956	Pa×s	691.86	Joback Method
dvisc	0.0022490	Pa×s	757.40	Joback Method
dvisc	0.0019314	Pa×s	822.94	Joback Method
dvisc	0.0016963	Pa×s	888.47	Joback Method
dvisc	0.0015166	Pa×s	954.01	Joback Method

Sources

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=U339772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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