Glutaric acid, 2-(adamant-1-yl)ethyl cyclohexylmethyl ester

Inchi: InChI=1S/C24H38O4/c25-22(7-4-8-23(26)28-17-18-5-2-1-3-6-18)27-10-9-24-14-19-11-20

InchiKey: CDHNNAUVDMDIQF-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-135.24	kJ/mol	Joback Method
hf	-766.83	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.430		Crippen Method
mcvol	320.460	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	3079.00		NIST Webbook
rinpol	3079.00		NIST Webbook
tb	940.71	K	Joback Method
tc	1164.97	K	Joback Method
tf	581.90	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1175.02	J/mol×K	940.71	Joback Method
cpg	1198.85	J/mol×K	978.09	Joback Method
cpg	1222.24	J/mol×K	1015.46	Joback Method
cpg	1245.41	J/mol×K	1052.84	Joback Method
cpg	1268.57	J/mol×K	1090.22	Joback Method
cpg	1291.93	J/mol×K	1127.60	Joback Method
cpg	1315.73	J/mol×K	1164.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405385&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