Glutaric acid, 3,5-dinitro-2-methylbenzyl isobutyl ester

Inchi: InChI=1S/C17H22N2O8/c1-11(2)9-26-16(20)5-4-6-17(21)27-10-13-7-14(18(22)23)8-15(1

InchiKey: HAADFHKFJZFNJA-UHFFFAOYSA-N

Formula: C17H22N2O8

SMILES: Cc1c(COC(=O)CCCC(=O)OCC(C)C)cc([N+](=O)[O-])cc1[N+](=O)[O-]

Mol. weight [g/mol]: 382.37

Physical Properties

Property code	Value	Unit	Source
gf	-223.40	kJ/mol	Joback Method
hf	-708.49	kJ/mol	Joback Method
hfus	57.43	kJ/mol	Joback Method
hvap	108.80	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	3.224		Crippen Method
mcvol	276.350	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	2832.00		NIST Webbook
tb	1085.80	K	Joback Method
tc	1334.96	K	Joback Method
tf	761.87	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.37	J/mol×K	1085.80	Joback Method
cpg	904.91	J/mol×K	1127.33	Joback Method
cpg	910.90	J/mol×K	1168.85	Joback Method
cpg	915.35	J/mol×K	1210.38	Joback Method
cpg	918.29	J/mol×K	1251.90	Joback Method
cpg	919.74	J/mol×K	1293.43	Joback Method
cpg	919.73	J/mol×K	1334.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377016&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume