Ethylene glycol bis(3,5-dinitrobenzoate)

Inchi: InChI=1S/C16H10N4O12/c21-15(9-3-11(17(23)24)7-12(4-9)18(25)26)31-1-2-32-16(22)1
InchiKey: FKERDMUSSICEEN-UHFFFAOYSA-N
Formula: C16H10N4O12
SMILES: O=C(OCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)c1cc([N+](=O)[O-])cc([N+](=O)[O
Mol. weight [g/mol]: 450.27
CAS: 60317-39-7

Physical Properties

Property code	Value	Unit	Source
gf	-55.50	kJ/mol	Joback Method
hf	-479.03	kJ/mol	Joback Method
hfus	74.74	kJ/mol	Joback Method
hvap	143.09	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	2.333		Crippen Method
mcvol	273.340	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	1398.70	K	Joback Method
tc	1713.74	K	Joback Method
tf	1091.76	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.88	J/mol×K	1398.70	Joback Method
cpg	801.66	J/mol×K	1451.21	Joback Method
cpg	792.58	J/mol×K	1503.71	Joback Method
cpg	781.72	J/mol×K	1556.22	Joback Method
cpg	769.13	J/mol×K	1608.73	Joback Method
cpg	754.89	J/mol×K	1661.24	Joback Method
cpg	739.08	J/mol×K	1713.74	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=C60317397&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
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

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