Decyl 4-nitrophenyl ether

Inchi: InChI=1S/C16H25NO3/c1-2-3-4-5-6-7-8-9-14-20-16-12-10-15(11-13-16)17(18)19/h10-13
InchiKey: FQIOGTJBANMZNX-UHFFFAOYSA-N
Formula: C16H25NO3
SMILES: CCCCCCCCCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 279.37
CAS: 31657-37-1

Physical Properties

Property code	Value	Unit	Source
gf	117.17	kJ/mol	Joback Method
hf	-291.49	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	73.15	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.114		Crippen Method
mcvol	235.830	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
tb	771.40	K	Joback Method
tc	981.81	K	Joback Method
tf	474.86	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.75	J/mol×K	771.40	Joback Method
cpg	716.03	J/mol×K	806.47	Joback Method
cpg	731.26	J/mol×K	841.54	Joback Method
cpg	745.47	J/mol×K	876.61	Joback Method
cpg	758.70	J/mol×K	911.68	Joback Method
cpg	770.99	J/mol×K	946.74	Joback Method
cpg	782.38	J/mol×K	981.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31657371&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume