Sebacic acid, decyl 2-nitrophenyl ester

Inchi: InChI=1S/C26H41NO6/c1-2-3-4-5-6-9-12-17-22-32-25(28)20-13-10-7-8-11-14-21-26(29)
InchiKey: BKOBZBLSPVDZAP-UHFFFAOYSA-N
Formula: C26H41NO6
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 463.61

Physical Properties

Property code	Value	Unit	Source
gf	-161.47	kJ/mol	Joback Method
hf	-855.27	kJ/mol	Joback Method
hfus	73.68	kJ/mol	Joback Method
hvap	111.31	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.305		Crippen Method
mcvol	385.740	ml/mol	McGowan Method
pc	921.62	kPa	Joback Method
rinpol	3573.00		NIST Webbook
tb	1130.36	K	Joback Method
tc	1391.66	K	Joback Method
tf	709.65	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1352.87	J/mol×K	1130.36	Joback Method
cpg	1366.29	J/mol×K	1173.91	Joback Method
cpg	1377.80	J/mol×K	1217.46	Joback Method
cpg	1387.51	J/mol×K	1261.01	Joback Method
cpg	1395.51	J/mol×K	1304.56	Joback Method
cpg	1401.89	J/mol×K	1348.11	Joback Method
cpg	1406.74	J/mol×K	1391.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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