

Sebacic acid, ethyl 2-nitro-4-chlorobenzyl ester

Inchi:	InChI=1S/C19H26ClNO6/c1-2-26-18(22)9-7-5-3-4-6-8-10-19(23)27-14-15-11-12-16(20)1
InchiKey:	NCBXTJRIHRCHLP-UHFFFAOYSA-N
Formula:	C19H26ClNO6
SMILES:	CCOC(=O)CCCCCCCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	399.87

Physical Properties

Property code	Value	Unit	Source
gf	-241.97	kJ/mol	Joback Method
hf	-738.00	kJ/mol	Joback Method
hfus	59.36	kJ/mol	Joback Method
hvap	100.78	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	4.975		Crippen Method
mvol	299.350	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2895.00		NIST Webbook
rinpol	2895.00		NIST Webbook
tb	1012.61	K	Joback Method
tc	1243.24	K	Joback Method
tf	673.20	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.42	J/molxK	1012.61	Joback Method
cpg	959.47	J/molxK	1051.05	Joback Method
cpg	969.17	J/molxK	1089.49	Joback Method
cpg	977.55	J/molxK	1127.93	Joback Method
cpg	984.64	J/molxK	1166.36	Joback Method
cpg	990.48	J/molxK	1204.80	Joback Method
cpg	995.09	J/molxK	1243.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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